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**CHARACTERIZATION OF SPHERES  
WITH THE SUBMICRON PARTICLE ANALYZER: FEASIBILITY**

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**RESEARCH DIRECTORATE**

**September 1992**

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CHARACTERIZATION OF SPHERES  
WITH THE SUBMICRON PARTICLE ANALYZER: FEASIBILITY

1. INTRODUCTION

The Submicron Particle Analyzer (SPA) is an instrument built by Wyatt Technology Corporation (Santa Barbara, CA) for the U.S. Army Chemical Research, Development and Engineering Center (CRDEC) that is used to study light scattering by aerosol particles.<sup>1,2</sup> The SPA comprises a spherical chamber in the center of which a dilute vertical stream of sampled aerosol particles traverses an intense horizontal laser beam, one particle at a time. Light scattered from each particle is intercepted and measured via 22 optical fibers that are distributed on the surface of the sphere and lead to 22 photomultiplier tubes and associated electronics in a separate instrument rack. The optical fibers, which are terminated on the chamber end with SELFOC gradient index lens, can be deployed among any of 72 ports on the sphere; the same nine port scattering angles are repeated along eight semi-great circles that are 45 degrees apart. The function of the SPA is to gather a set of light scattering data from each aerosol particle, from which physical characteristics of the particles (i.e., size and shape) may be inferred. The aim of our current research with this instrument is to work out the appropriate types of data to be included in the measured sets and to discover the manner in which those data sets may be manipulated to reveal desired particle characteristics.

Light scattering instruments built for sizing spherical particles typically measure scattered intensity in one or two directions and produce a "signal" proportional to either an intensity or a ratio of intensities. These instruments differ according to the scattering and acceptance angles chosen and the spectral nature of the illuminating radiation. In any case, a response curve is calculated that gives the signal level expected as a function of particle diameter; often, a calibration with a few spheres of known size is also required to match calculated and actual signals. There are several well-known problems with this approach. First, it is the nature of scattering by spheres that the response curves are not single valued -- that is, there are several sizes of spheres that can produce any given signal level. This effect may be mitigated, but never completely eliminated, by choices made in the instrument's design. Also, the response curve depends on the refractive index of the sphere; therefore, a different curve and calibration, if necessary, must be available for every different particle material. In practice, this is rarely done. Finally, these instruments provide no way to check whether each scattering particle is actually a sphere. The spherical response curve is simply applied to every particle that scatters light whether it is appropriate or not.

With the SPA and its multiplicity of light scattering channels, we may have an opportunity to design a measurement and analysis technique that will characterize spherical particles with a confidence never before attained. In this report, we will propose a direct inversion technique for processing SPA data, write the necessary computer codes to implement the technique, and then test the procedure using computer-generated, synthetic data to represent

experimental measurements that can be collected with the SPA. We wish to discover whether a useful characterization of spherical particles is feasible given the nature and accuracy of SPA light scattering data.

## 2. OUTLINE OF THE INVERSION METHOD

In the context of the present problem, an inversion method may be said to be successful when it produces estimates for the size and refractive index of a sphere such that the calculated light scattering properties of that particular sphere agree with the corresponding measured properties. A formal mathematical inverse solution to the MIE equations, to express size parameter ( $x$ ) and refractive index ( $n$ ) in terms of scattering intensities, is not possible. Instead, we shall discover acceptable values for  $x$  and  $n$  by considering, one pair at a time, all possible values of  $x$  and  $n$ , repeatedly asking if the spheres specified by the  $x, n$  pairs scatter light in agreement with the measurements, and noting the ones that do. The phrases "all possible values" and "in agreement with the measurements" require some elaboration.

### 2.1 N-X Plane.

In principle, there are an infinite number of possible values of  $x$  and  $n$ , so the range of those variables necessarily must be restricted. A large majority of dielectric materials, both liquids and solids, have refractive indices between 1.3 and 1.8 at visible wavelengths, and so that range is selected. (Absorbing spheres, in contrast with dielectric ones, must be characterized with a third parameter in addition to  $x$  and  $n$ , and are consequently beyond the scope of this report.) The size parameters considered will be restricted to the range  $0 < x \leq 10$ , though with less clear justification; inversion of scattering from small particles should be more reliable owing to their simpler scattering patterns; whereas, a maximum size parameter of 10 -- corresponding in blue light to a physical diameter of about  $1.6 \mu\text{m}$  -- is large enough to include many standard particles available for experiments.

Therefore, as a starting point, we consider spheres represented by their coordinates on the  $x$ - $n$  plane in the region  $0 < x \leq 10$  and  $1.3 \leq n \leq 1.8$ . The region is divided into a number of much smaller rectangular areas (pixels) of dimensions  $\Delta x$  and  $\Delta n$ , with the aim of letting the sphere described by the central coordinates of each pixel stand for all the spheres represented within that pixel. This scheme succeeds if the relevant scattering properties of central spheres in adjacent pixels differ by less than the expected experimental uncertainty. Clearly, the pixel resolution must be at least as small as the accuracy with which we wish to recover  $x$  and  $n$ . However, the finer the resolution, the lengthier the inversion calculation, and there is no point in demanding a higher resolution than that which can be supported by the experimental accuracy. None of these factors are known a priori; to get started, we choose, rather arbitrarily,  $\Delta x = .05$  and  $\Delta n = .005$ . This results in an array of 20,200 pixels stacked in 200 columns centered at  $x = 0.05, 0.10, \dots 10.00$ , and along 101 rows centered at  $n = 1.300, 1.305, \dots 1.800$ .

Although the pixels represent a 2-dimensional array (the  $x$ - $n$  plane), it will be convenient for later purposes to name the pixels with a

single, rather than a double, index. The pixel in the lower left corner  $(x,n) = (0.05, 1.300)$  is pixel number 1; that in the lower right corner  $(10.00, 1.300)$  is number 200, etc., left to right and up the rows to pixel number 20,200 in the upper right corner  $(10.00, 1.800)$

## 2.2 Selection of Scattering Properties.

The nature of the experimentally observable quantities, which will be compared to their calculated values for each sphere, must now be specified. As noted in Section 1 of this report, the SPA allows 22 intensities to be recorded for each particle. The laser beam intensity profile is Gaussian; since the exact path of particles through the beam is uncontrollable, the incident beam intensity for any particle is unknown, and the absolute values of the scattered intensities have little meaning. The ratios among the various scattered intensities for each particle are independent of the incident beam and can serve as the light scattering properties for inversion. Since all the detector SELFOC lenses have the same apertures and are equidistant from the scattering particle, we may refer to the observable quantities interchangeably as either intensity ratios or flux ratios.

To distinguish spherical from nonspherical particles, eight detectors, without polarizers, are placed in a ring at a scattering angle of  $\theta = 55^\circ$ , and the incident beam is prepared in a right circularly polarized state. For spherical particles illuminated in this way, there can be no variation of light scattering with azimuth angle,  $\phi$ ; uniformity of the eight detector signals confirms particle sphericity. Random experimental noise will preclude exact equality of the eight measurements even for perfect spheres. However, the standard deviation will be small and the average value, owing to the eight times sampling, provides an excellent reference figure for forming ratios. The average intensity measurement of these eight ring detectors will be the denominator in every intensity ratio.

Eight equivalent (scattering independent of  $\phi$  for spheres) detector ports are available at each of the remaining eight scattering angles:  $\theta = 10, 40, 75, 90, 105, 125, 140, \text{ and } 170^\circ$ . At any port, the scattered light may be detected through either a linear polarizer in one of two orientations or without a polarizer at all. There are then 64 ports through which up to 24 different measurements may be made and ratioed to the  $\theta = 55^\circ$  measurement to form 24 scattering properties of the particle. Only 14 of the original 22 detectors remain available; therefore, a 14-member subset of the 24 possible ratios must be chosen. The final selection will be discussed in Section 3.4 of this report.

## 2.3 Pixel Acceptance Criterion.

Preliminary calculations and plots to assess the character of flux ratios over the  $x$ - $n$  plane revealed a deficiency in the original plan that divided the plane into pixels with sides  $\Delta x = .05$  and  $\Delta n = .005$ . There are regions that correspond to morphology-dependent resonances<sup>3</sup> of the sphere where the flux ratio grows rapidly to several times its value in neighboring pixels. Figure 1 shows the value of one flux ratio over a line in the  $x$ - $n$  plane defined by  $n = 1.75$  and  $9.3 \leq x \leq 9.6$ . This particular ratio happens to

be the intensity received through a horizontal polarizer at  $\theta = 90^\circ$  to (as always) the intensity received through no polarizer (unpolarized) at  $\theta = 55^\circ$ . The heavy vertical lines represent pixel boundaries in the x direction, and the dots correspond to the pixel centers, at (9.30, 1.75), (9.35, 1.75), ..., (9.60, 1.75).

The amplitude of the ratio can vary by a factor of four or more across a single pixel of this size ( $\Delta x = .05$ ) in the vicinity of a resonance; clearly, no single ratio value can adequately represent so large a domain. One obvious cure is to reduce the pixel size; however, judging from the steepest slope in Figure 1, it is estimated that the pixel dimension must be reduced to about  $\Delta x = .001$ , 50 times smaller than present, to ensure that the ratio varies by no more than 5% across the x-dimension of any pixel. A reduction in  $\delta\lambda$  by a similar factor would also be required, resulting in a network of some 50 million pixels over the area of the x-n plane now covered by about 20 thousand. The inefficiency in designing everywhere for the worst-case condition (up the slope of a resonance) would be colossal; in any event, the enormous demands on computer memory and central processing unit time prohibit this approach.

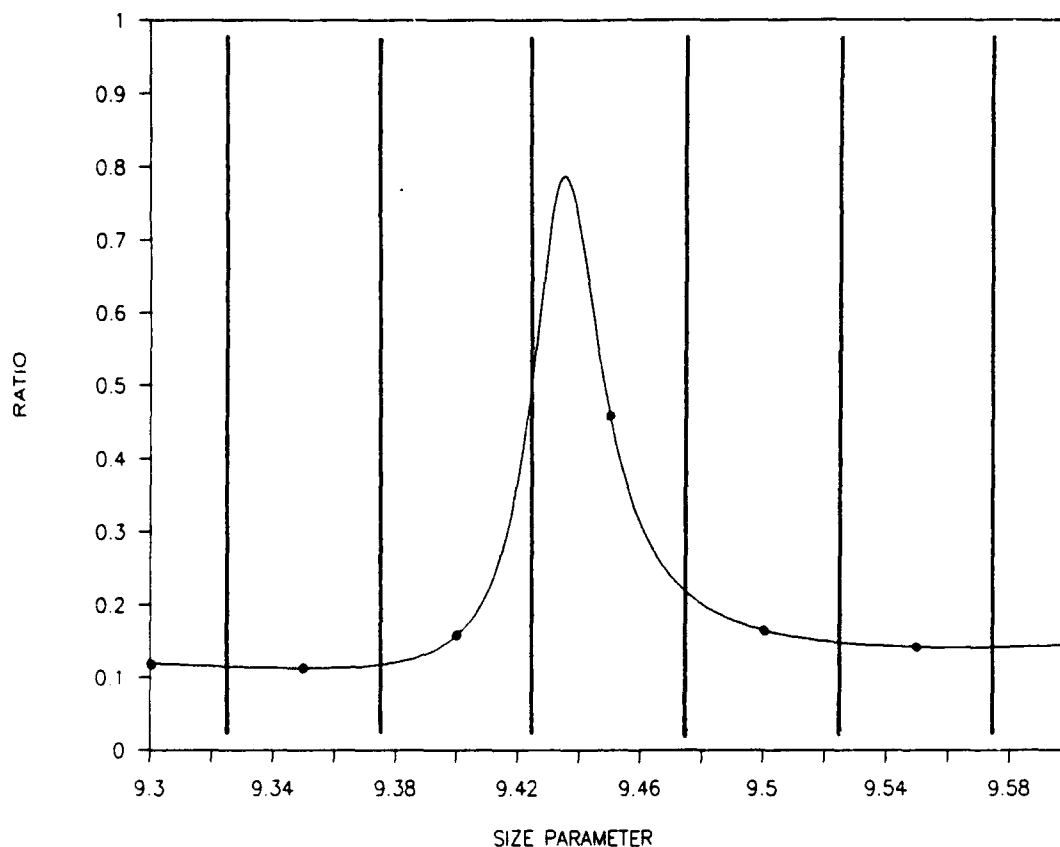


Figure 1. Detailed View of the H090 Flux Ratio Over a Segment of the X,N Plane

Instead, we leave the pixel dimensions unchanged and record for each pixel the minimum and maximum values of the flux ratios over all the pixel, not just the ratio values at the center of the pixel. This doubles the amount of data that must be made available to the inversion program, but that is all. This method will give correct, if not necessarily useful, results with pixels of any dimensions that may be chosen later on.

Each flux ratio determined with the SPA will have an experimental uncertainty associated with it, depending on the absolute magnitude of the measured intensities. Establishing rules for estimating the uncertainty will be an important task in the experimental phase of this inversion project; however, for the present feasibility study, we may simply specify uncertainties as needed. The inversion process may be summarized as follows. Consider a single pixel and a single flux ratio: if the physical sphere's size and refractive index are given by any point (x,n) within the pixel, then the true flux ratio must lie between the calculated minimum and maximum flux ratios. The experimentally determined flux ratio is really a range of ratios from (Measurement - Uncertainty) to (Measurement + Uncertainty). If the calculated and experimental ranges overlap, the pixel may contain the sphere's actual size and refractive index. If there is no overlap, the pixel cannot contain the sphere's parameters. After all the flux ratios have been checked in this manner over a pixel, that pixel may be reported as an inversion solution if agreement occurred for every flux ratio. If at least in principle even one pair of calculated and measured flux ratios failed to overlap, the pixel is to be rejected.

### 3. CALCULATION OF SCATTERED INTENSITIES

#### 3.1 Scattered Intensity at a Point.

Consider a plane wave incident on an isolated single particle as shown in Figure 2 and ignore for the moment the indicated polarizer. The Stokes vector of the scattered light falling onto an infinitesimally small aperture in the direction  $\theta$  and located a distance R from the particle is given by<sup>4</sup>

$$\begin{pmatrix} I_s \\ Q_s \\ U_s \\ V_s \end{pmatrix} = \frac{1}{k^2 R^2} \begin{pmatrix} S_{11} & S_{12} & S_{13} & S_{14} \\ S_{21} & S_{22} & S_{23} & S_{24} \\ S_{31} & S_{32} & S_{33} & S_{34} \\ S_{41} & S_{42} & S_{43} & S_{44} \end{pmatrix} \begin{pmatrix} I_i \\ Q_i \\ U_i \\ V_i \end{pmatrix} \quad [\text{watt/cm}^2] \quad (1)$$

where  $I_i$ ,  $Q_i$ ,  $U_i$ , and  $V_i$  are the Stokes parameters of the incident beam and  $k = 2\pi/\lambda$ . Each Stokes parameter has the dimension of intensity (e.g., watts/cm<sup>2</sup>), whereas, the 16 scattering matrix elements  $S_{ij}$  are dimensionless and functions of  $\theta$ .

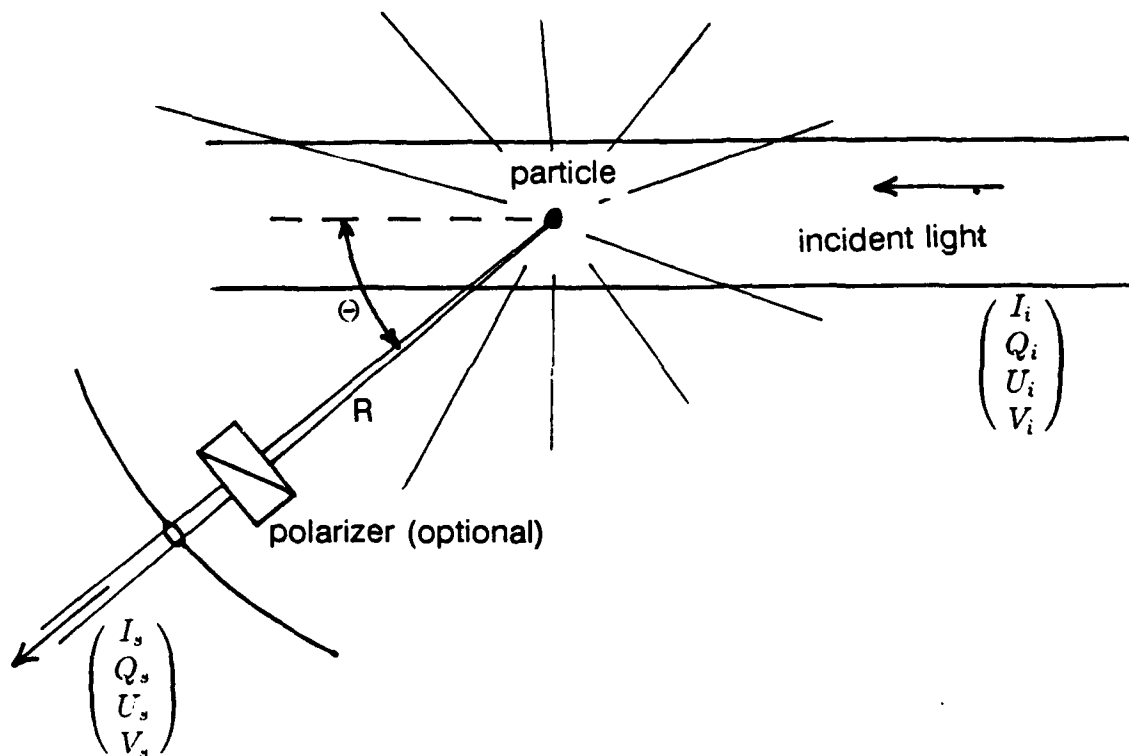


Figure 2. Light Scattering Geometry of the Submicron Particle Analyzer

In the particular case where the particle is spherically symmetric and the incident beam is right circularly polarized and of intensity  $I_0$ , equation 1 simplifies to the form

$$\begin{pmatrix} I_s \\ Q_s \\ U_s \\ V_s \end{pmatrix} = \frac{1}{k^2 R^2} \begin{pmatrix} S_{11} & S_{12} & 0 & 0 \\ S_{12} & S_{11} & 0 & 0 \\ 0 & 0 & S_{33} & S_{34} \\ 0 & 0 & -S_{34} & S_{33} \end{pmatrix} I_0 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad (2)$$

The Stokes vector of the scattered light is then

$$\begin{pmatrix} I_s \\ Q_s \\ U_s \\ V_s \end{pmatrix} = \frac{I_0}{k^2 R^2} \begin{pmatrix} S_{11} \\ S_{12} \\ S_{34} \\ S_{33} \end{pmatrix} \quad (3)$$

and the intensity of the scattered light (i.e., the first Stokes parameter) falling upon the aperture is

$$I_s = \frac{I_0}{k^2 R^2} S_{11} \quad (4)$$

Let an ideal linear polarizer be placed in front of the aperture with its transmission axis oriented at an angle  $\rho$  with respect to the scattering plane -- the plane containing the aperture and the incident beam. When the polarizer transmission axis is parallel to the scattering plane,  $\rho = 0^\circ$ . The angle grows positively as the polarizer is rotated counterclockwise, as seen by an observer looking inward through the aperture. With the polarizer inserted, the Stokes vector of scattered light reaching the aperture is given by

$$\begin{pmatrix} I_s \\ Q_s \\ U_s \\ V_s \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & \cos 2\rho & \sin 2\rho & 0 \\ \cos 2\rho & \cos^2 2\rho & \cos 2\rho \sin 2\rho & 0 \\ \sin 2\rho & \cos 2\rho \sin 2\rho & \sin^2 2\rho & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \times \frac{1}{k^2 R^2} \begin{pmatrix} S_{11} & S_{12} & 0 & 0 \\ S_{12} & S_{11} & 0 & 0 \\ 0 & 0 & S_{33} & S_{34} \\ 0 & 0 & -S_{34} & S_{33} \end{pmatrix} I_0 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad (5)$$

After multiplying the factors in equation 5, we find the intensity falling on the small aperture as

$$I_s = \frac{I_0}{2k^2 R^2} (S_{11} + S_{12} \cos 2\rho + S_{34} \sin 2\rho) \quad (6)$$

Two polarizer orientations lead to simple results. When the polarizer is oriented horizontally ( $\rho = 0^\circ$ ), the intensity is proportional to  $S_{11} + S_{12}$ ; if it is oriented diagonally ( $\rho = 45^\circ$ ), then the intensity is proportional to  $S_{11} + S_{34}$ . It is impossible to bring an explicit  $S_{33}$  dependence to the scattered light in this configuration; however, the scattering matrix elements for a sphere are related by<sup>5</sup>

$$S_{11}^2 = S_{12}^2 + S_{34}^2 + S_{33}^2 \quad (7)$$

so that, except for its sign, the  $S_{33}$  element is implicitly determined when the other three elements are determined.

Letting subscripts H, D, and U represent the cases of horizontal polarizer, diagonal polarizer, and no polarizer, respectively, the following equation summarizes the results of this section and gives the intensity of the scattered light reaching an infinitesimal aperture at scattering angle  $\theta$

$$\begin{aligned} IU(\theta) &= \frac{I_0}{2k^2 R^2} [S_{11}(\theta) + S_{11}(\theta)] \\ IH(\theta) &= \frac{I_0}{2k^2 R^2} [S_{11}(\theta) + S_{12}(\theta)] \\ ID(\theta) &= \frac{I_0}{2k^2 R^2} [S_{11}(\theta) + S_{34}(\theta)] \end{aligned} \quad (8)$$



### 3.2 Correction for Finite Acceptance Angle.

If the intensity of light "I," perpendicularly incident on an aperture of area "A," is constant over its surface, then the flux through the aperture is simply  $IA$ . However, if the intensity varies with position on the aperture, an integration is required to find the total flux.

Figure 3 shows a circular aperture of radius  $r$  (representing the clear opening of one of the SELFOC lens collecting scattered light in the SPA) located a distance  $R$  away from the scatterer in the direction  $\theta_0$ . The intensity of the scattered light reaching the aperture varies with  $\theta$  (only), as is suggested by the figure's shading.

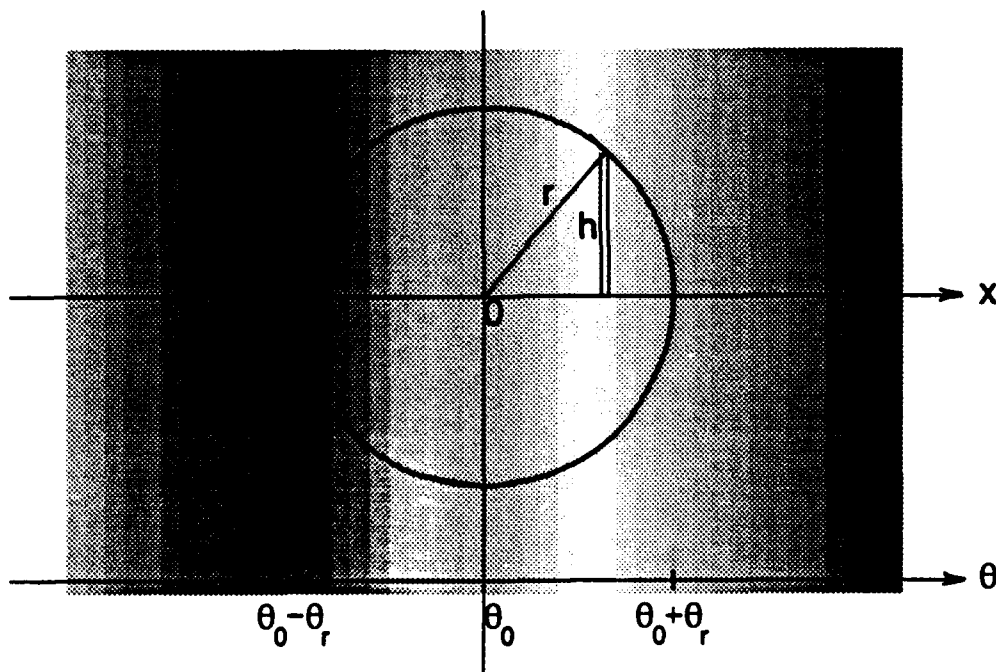


Figure 3. Scattered Light of Varying Intensity Falling on a SELFOC Fiber-Optic Lens

Since  $x = R (\theta - \theta_0)$  and  $dx = R d\theta$ , the total flux through the circular aperture is given by

$$F = \int_{\theta_0 - \theta_r}^{\theta_0 + \theta_r} I(\theta) 2h(\theta) R d\theta \quad (9)$$

The height  $h$  satisfies

$$r^2 = x^2 + h^2 = R^2(\theta - \theta_0)^2 + h^2 \quad (10)$$

and so

$$F = \int_{\theta_0 - \theta_r}^{\theta_0 + \theta_r} 2R^2 I(\theta) \sqrt{\theta_r^2 - (\theta - \theta_0)^2} d\theta \quad (11)$$

If the expressions for  $I(\theta)$  (equation 8) are substituted into equation 11, the resulting integral cannot be evaluated analytically owing to the complexity of the  $S_{ij}$ . A tractable approximation to  $I(\theta)$  can be derived by evaluating  $I(\theta)$  at a set of discrete angles in the vicinity of the aperture and interpolating linearly between the calculated values. The SELFOC lenses have a clear diameter of 1.8 mm and are located 93 mm from the center of the SPA chamber; therefore,  $\theta_r = .9/93 = .00968$  radians, or  $0.55^\circ$ . The computer program (described Section 3.3) can calculate the  $S_{ij}$  at intervals of one degree or greater, and the lenses are centered on integral degree values. Figure 4 shows the situation approximately to scale.

From Figure 4, we see that  $I(\theta)$  to the left of  $\theta_0$  is given by the straight line whose equation is

$$I(\theta) = \frac{I(\theta_0) - I(\theta_0 - d)}{d} [\theta - (\theta_0 - d)] + I(\theta_0 - d) \quad (12)$$

while for  $\theta \geq \theta_0$

$$I(\theta) = \frac{I(\theta_0 + d) - I(\theta_0)}{d} [\theta - (\theta_0)] + I(\theta_0) \quad (13)$$

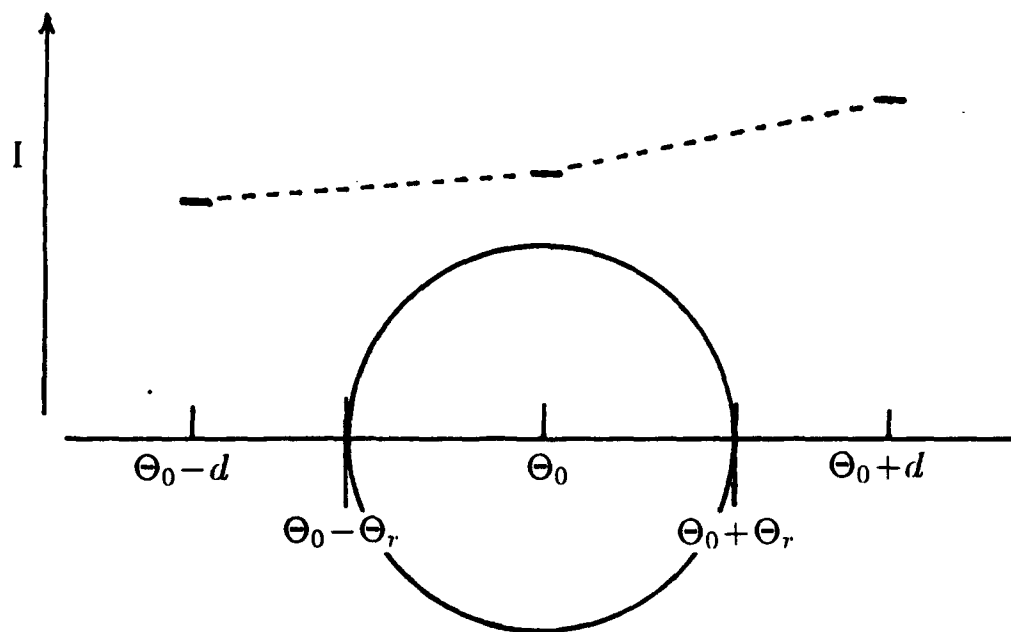


Figure 4. Calculation, at One Degree Intervals, of Light Scattering in the Vicinity of a SELFOC Lens

Substituting equations 12 and 13 into equation 11 gives the total flux through the aperture as

$$\begin{aligned}
 F = 2R^2 \int_{\theta_0 - \theta_r}^{\theta_0} \sqrt{\theta_r^2 - (\theta - \theta_0)^2} \left\{ \frac{I(\theta_0) - I(\theta_0 - d)}{d} [\theta - (\theta_0 - d)] + I(\theta_0 - d) \right\} d\theta \\
 + 2R^2 \int_{\theta_0}^{\theta_0 + \theta_r} \sqrt{\theta_r^2 - (\theta - \theta_0)^2} \left\{ \frac{I(\theta_0 + d) - I(\theta_0)}{d} [\theta - (\theta_0)] + I(\theta_0) \right\} d\theta
 \end{aligned} \tag{14}$$

Making a change of variable to  $\phi = \theta - \theta_0$  simplifies the expression to

$$\begin{aligned}
 F = 2R^2 \left\{ \frac{I(\theta_0) - I(\theta_0 - d)}{d} \int_{-\theta_r}^0 \sqrt{\theta_r^2 - \phi^2} (\phi + d) d\phi + I(\theta_0 - d) \int_{-\theta_r}^0 \sqrt{\theta_r^2 - \phi^2} d\phi \right\} \\
 + 2R^2 \left\{ \frac{I(\theta_0 + d) - I(\theta_0)}{d} \int_0^{\theta_r} \sqrt{\theta_r^2 - \phi^2} \phi d\phi + I(\theta_0) \int_0^{\theta_r} \sqrt{\theta_r^2 - \phi^2} d\phi \right\}
 \end{aligned} \tag{15}$$

The integrals in equation 15 are readily evaluated; after some algebra, the flux equation reduces to

$$F = \pi \theta_r^2 R^2 \left[ \frac{2\theta_r}{3\pi d} I(\theta_0 - d) + \left( 1 - \frac{4\theta_r}{3\pi d} I(\theta_0) \right) + \frac{2\theta_r}{3\pi d} I(\theta_0 + d) \right] \tag{16}$$

This equation takes the simple form

$$F = \pi \theta_r^2 R^2 I(\theta_0) \quad (17)$$

as expected when  $\theta_r$  goes to zero or when all three intensities are set equal to  $I(\theta_0)$ .

When the numerical values for  $\theta_r$  and  $d$  are substituted (.55 and  $1^\circ$ ), we find

$$F = \pi \theta_r^2 R^2 [ .1175 I(\theta_0 - 1^\circ) + .7650 I(\theta_0) + .1175 I(\theta_0 + 1^\circ) ] \quad (18)$$

which gives the proportions for combining the intensity at the nominal detector angle with the intensities calculated one degree before and after that angle to correct for the finite acceptance angle of the SELFOC lenses. The correction makes little difference for spheres in the size range of interest because the intensity is quite a slow varying function of scattering angle for these small particles; however, for completeness and safety, the correction will be included in the intensity calculations that follow.

### 3.3 Mie Computer Programs.

The expression of the quantities  $S_{ij}$  (scattering matrix elements in equations 2 through 8) in terms of the size and refractive index of spheres is the subject of Mie theory, which is discussed in detail in the standard texts of light scattering.<sup>4,6,7,8</sup> The Mie equations are quite complex and are evaluated by computer to yield up numerical values for the scattering matrix elements.

The computer program adapted for this project was distributed several years ago by Peter Barber, now at Clarkson University (Potsdam, NY), and is named, appropriately, MIE. MIE calculates various light scattering functions for homogeneous spheres and is based on the original program by Dave,<sup>9</sup> later expanded upon by Wiscombe.<sup>10</sup> MIE requests as input the size parameter and real and imaginary parts of the sphere's refractive index and the desired angular increment (1, 2, 3, 5, and  $10^\circ$  are allowed) at which calculations are to be performed. The output is written to a file named SPHERE.DAT, and comprises a few lines repeating the input data and displaying calculated efficiencies, followed by seven columns of data headed with the following titles: ANGLE, M SUB 2, M SUB 1, S SUB 21, D SUB 21, INTENSITY, and POLAR.

The scattering ANGLES run from 0 to 180 °, inclusively, in steps of the specified increment. The next four columns relate to the scattering matrix elements as

$$\begin{aligned}\frac{1}{2}(M \text{ SUB } 2 + M \text{ SUB } 1) &= S_{11} \\ \frac{1}{2}(M \text{ SUB } 2 - M \text{ SUB } 1) &= S_{12} \\ S \text{ SUB } 21 &= S_{33} \\ D \text{ SUB } 21 &= S_{34}\end{aligned}\tag{19}$$

The sixth and seventh columns are useful combinations of previous ones, namely

$$\begin{aligned}\text{INTENSITY} &= \frac{1}{2} (M \text{ SUB } 2 + M \text{ SUB } 1) \quad (= S_{11}) \\ \text{POLAR} &= \frac{(M \text{ SUB } 2 - M \text{ SUB } 1)}{(M \text{ SUB } 2 + M \text{ SUB } 1)} \quad \left(= \frac{S_{12}}{\text{INTENSITY}}\right)\end{aligned}\tag{20}$$

The heart of Barber's MIE program<sup>3</sup> is the subroutine SMIE, which does the actual evaluation of the quantities M SUB 2, etc. The input parameters, or functions derived from them, are passed to SMIE, which then returns a 3-dimensional array called ELTRMX(I,J,K) to the calling program.

The index I (~ 1,4) specifies the type of scattering function in each element of the array, according to

$$\begin{aligned}1 &\sim M \text{ SUB } 2 \\ 2 &\sim M \text{ SUB } 1 \\ 3 &\sim S \text{ SUB } 21 \\ 4 &\sim D \text{ SUB } 21\end{aligned}\tag{21}$$

The indices J (= 1, (90/D)+1) and K (= 1,2), together, specify the scattering angle appropriate to each element of the array, given D, the increment between scattering angles. The relations between  $\theta$ , D, J, and K are

$$\begin{aligned} \theta &= D(J-1) && \text{when } K = 1, \quad (0 \leq \theta \leq 90^\circ) \\ \text{and } \theta &= 180^\circ - D(J-1) && \text{when } K = 2, \quad (91^\circ \leq \theta \leq 180^\circ) \end{aligned} \quad (22)$$

This subroutine SMIE is used, unaltered, in my program HILO.F for calculating the data sets of flux ratios.

#### 3.4 Calculation of the Flux Ratio Data Sets: HILO.F.

All elements have now been assembled to write a program to calculate the minimum and maximum values of each flux ratio over each pixel in the x-n plane. Looking ahead to the results of the calculation, when a 3-D surface plot is made of any of these flux ratios over the x-n plane (Figures 5 and 6 of the main body of this report and Appendix B), a landscape is revealed of nearly parallel valleys and sharply rimmed ridges. There are no pits or peaks in the flux ratio values -- apparent spikes along the tops of ridges are artifacts of the plotting program -- therefore, in virtually every case, the extreme of the flux ratio for a pixel will occur on the perimeter of the pixel. Occasionally, when an absolute valley bottom or ridge crest is attained on the plane, the slope at that point is very gentle in at least one direction; therefore, there is no significant difference between that interior minimum (or maximum) value and the minimum (or maximum) around the pixel's perimeter.

So, instead of calculating flux ratios at a high density of x,n points over the pixels, it suffices to perform the calculations only on the perimeter around each pixel. More time is saved by noting that each interior pixel edge is common to two pixels and, in most cases, only two edges per pixel need be calculated. By avoiding calculations at points internal to the pixel, we save computation time by a factor of nearly NSAMPS/2, where NSAMPS is the number of sampling points along one edge of a pixel. In the program HILO.F, NSAMPS is set equal to 6 in the left half of the plane and equal to 20 in the more steeply corrugated right half of the plane.

The source code for HILO.F is listed in Appendix A and is reasonably well self documented; an overview of its operation follows. The main program HILO selects pixels in order from left to right, one row at a time, beginning with the bottom row (n = 1.300), and on each pixel selects which of the four edges to evaluate. HILO calls subroutine SIDE once for each edge and specifies NSAMPS. SIDE calculates the values of x and n at the

sampling sites along the edge, and at each sampling site calls the subroutine SMIE. SMIE returns (to SIDE) the array ELTRMX, which holds scattering functions as a function of scattering angle (every one degree) for the site. SIDE then calls subroutine UDHINT, which computes the three intensities, IH, ID, and IU, for each of the nine SPA scattering angles (correcting for detector acceptance angle) and writes them to one column of the array IO. When IO is finally filled, it contains 27 rows and NSAMPS columns of intensities.

The intensities in IO are converted by SIDE to flux ratios by dividing each element in every row by the corresponding element in the row representing the reference intensity, namely the intensity scattered at 55° through no polarizer. Another array, MINMAX, is filled with values taken from IO; the smallest of the NSAMPS values in the kth row of IO is put into the first column of the kth row of MINMAX and the largest value of the same row goes in the second column. At the end, MINMAX is returned to HILO and contains the minimum and maximum values of each flux ratio over whichever pixel edge HILO originally requested.

Back in HILO, the contents of MINMAX are entered in a much larger 3-D array called ACCUM, which accumulates this edge data for all of the 200 pixels in the row. HILO keeps track of which edge data can be copied from an earlier calculation and which must be computed freshly. When ACCUM is filled, the four edges of each pixel are compared and the very smallest and largest flux ratio values for each pixel are appended to the output files. HILO then moves up to the next row of pixels and the process begins again.

Each output file comprises 20,200 lines, one for each pixel and in pixel order. A single real number specifying the minimum (or maximum) value attained by a particular flux ratio on the corresponding pixel is on each line. The files are named by describing the numerator flux with four characters. The first letter, one of H, D, or U indicates that the light either passed through a horizontally oriented polarizer, a diagonally oriented polarizer, or no polarizer, respectively, while the last three digits indicate the scattering angle. The extensions ".min" and ".max" are added to specify files of minimum and maximum flux ratios. There are 54 data files in all -- minimums and maximums for each of 3 polarizations at 9 scattering angles -- but of course two files, U055.MIN and U055.MAX, contain only 1.0's.

HILO was compiled and run on a Stardent minicomputer (Ardent Computer Corporation, Dobbs Ferry, NY) and required just over 5 hr to complete. The data sets were transferred to a personal computer, where the graphing program "Surfer" was used to prepare plots for visualizing the flux ratios. Figures 5 and 6 show typical data sets; the surfaces of minimum (Figure 5) and maximum (Figure 6) values of the flux ratio U090 were plotted over the x-n plane in both surface and contour formats. The true surface of U090 lies on or above the surface of U090.MIN and on or below the surface of U090.MAX. The regularly spaced spikes along mountain crests, especially evident in Figure 5, are plotting artifacts, which result because the sampling and plotting mesh of pixels is too coarse to represent the true knife-edge ridges. Actually, there are no points of relative maxima of U090 over the plotted part of the x-n plane, and only two relative minima I can find --



shallow valley bottoms indicated by closed contour loops at about  $(x,n) = (6.6,1.5)$  and  $(8.3,1.4)$ .

Plots of flux ratio maximum values, such as those in Figure 6, present a better picture of the true flux ratio than do plots of flux ratio minimum values. One can imagine that the upper plot of Figure 6 represents an opaque paint, covering - perhaps too thick at places - the flux ratio surface.

Surface plots of the maximum values of all the flux ratios are cataloged in Appendix B of this report. At scattering angles of 10 and 170°, there are few differences among the H, D, and U flux ratios (except for a factor of 2), which was expected. At 0 and 180°, the distinctions vanish altogether because  $S_{12} = S_{34} = 0$  (equation 8). Therefore, we would deploy detectors to measure, at the most, one of the three polarizations at those two extreme angles. Polarization-dependent differences among the flux ratios at more central scattering angles are much more apparent.

Graphs in Appendix B of this report allow us to envision the nature of the light scattering flux ratios, but they offer little guidance in selecting the optimum ratios to measure with the 14 available detectors. The problem is that contour lines for all the flux ratios follow the same patterns, which lay in similar directions along lines of  $n,x = \text{constant}$ . There are no data sets whose contours run perpendicular to the others, which, because of their orthogonality, would be especially important to include among the 14 measurements. Instead, we settled on data sets according to the following experimentally pragmatic criteria. Too much background light is picked up by detectors at 10 and 170°; until that can be corrected by redesigning the scattering chamber, no data will be collected at those angles. Generally, more light is available without a polarizer than through one; because higher intensity implies better signal to noise ratio, we take all the remaining unpolarized data sets (e.g., U040, U075, U090, U105, U125, and U140). At most scattering angles, the scattering through a horizontal polarizer seems to differ more from the unpolarized scattering than the scattering through a diagonal polarizer; therefore, we collect horizontal data sets at the same six scattering angles. This would leave room for two diagonally polarized data sets, which we take at 40 and 90°.

#### 4. TESTING THE INVERSION METHOD

##### 4.1 Program INVERT.

The FORTRAN program "INVERT" was written to explore and test the inversion procedure. INVERT first reads in a number of files, which includes the computed min/max values over the  $x$ - $n$  plane for the 14 selected flux ratios, a row of experimental detector calibration coefficients (used in this study to apply controlled errors to the synthetic input data), and the synthetic input data [an  $N$  by 24 array of numbers (EXPDAT??TST) generated in a separate program (DATGEN) and simulating SPA measurements on a run of  $N$  particles]. When inverting real data, the experimental uncertainty associated with each flux ratio measurement will be individually determined, based on the

U090.MIN

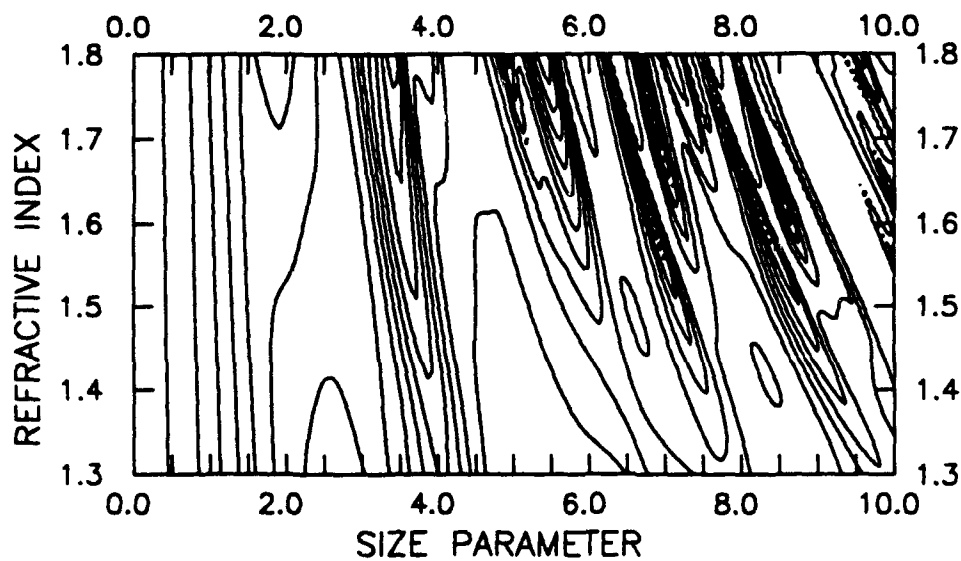
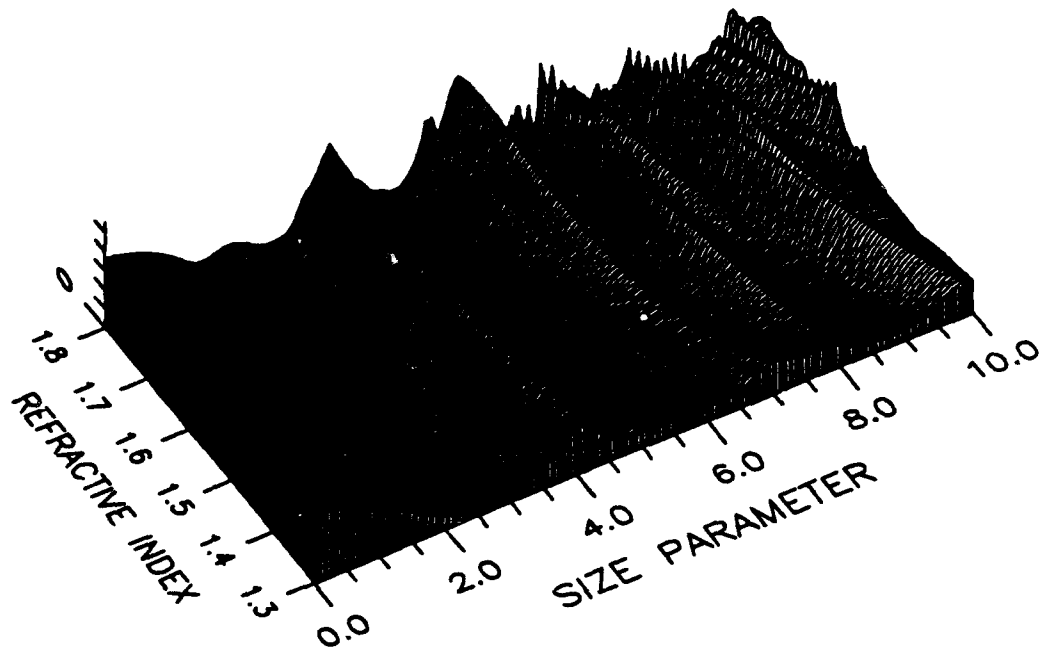


Figure 5. Surface of Pixel Minimum Values of the Flux Ratio U090 Over the X,N Plane

# U090.MAX

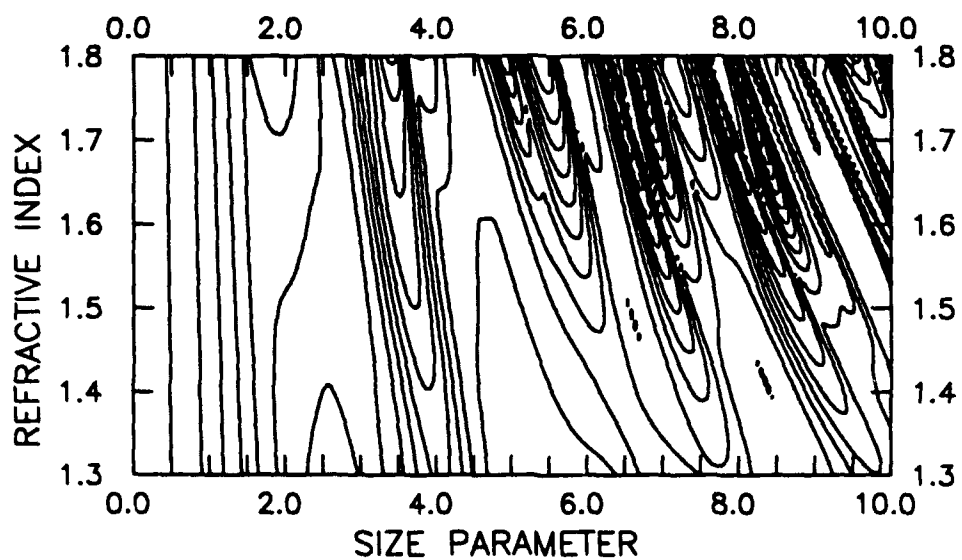
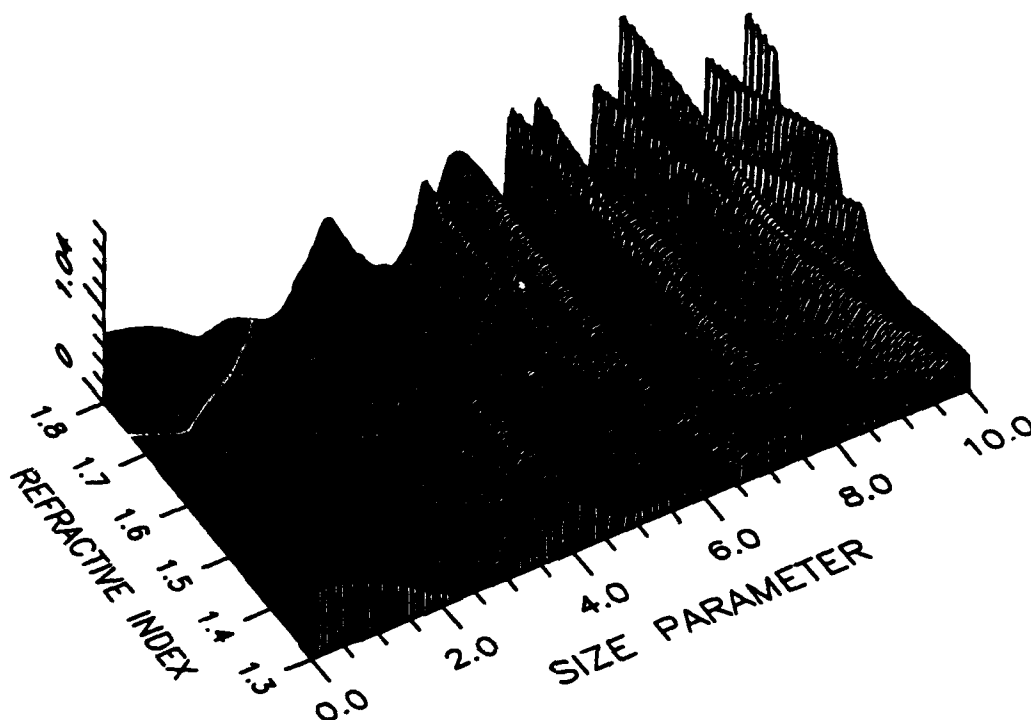


Figure 6. Surface of Pixel Maximum Values of the Flux Ratio U090 Over the X,N Plane

measured absolute scattering intensity. However, for this feasibility study, we have assigned a number of constant uncertainties to the flux ratios to observe their effect.

Taking one particle at a time (i.e., one row of EXPDAT??TST), INVERT computes the 55°-ring average intensity and the 14 flux ratios, and then expands the 14 flux ratios into measured flux ratio ranges (nominal value plus and minus the assigned uncertainty). On each pixel, INVERT must check for agreement (overlap) between the particle's "measured" range of ratio values and the previously calculated range of ratio values for each of the 14 flux ratios. This is accomplished with an algorithm (described in the following paragraph) that is much faster than literally asking 20,200 times for each of 14 flux ratios if an overlap occurs.

The 28 files of minimum and maximum flux ratios read in by INVERT are not exactly the files outputted by HILO -- U040.MIN and others. HILO files are first acted on by the program ORDERALL, which sorts each file in ascending order of flux ratio and simultaneously writes for each file an ancillary integer file that relates the original pixel order to the newly sorted order. The file U040.MIN, written by HILO, is renamed ORD\_U040.MIN when its data are sorted, and the corresponding integer file is named NDX\_U040.MIN; other files are analogously named. The files ORD\*. and NDX\*. (a total of 56) are read by INVERT during its initialization.

The method of determining if overlap occurs between a pixel's calculated range and the experimental range for a flux ratio and the motive for sorting the data files into ascending order are illustrated in Figure 7. In the upper half of Figure 7, the short horizontal bars represent the calculated minimum values of one of the 14 flux ratios; the shaded patches above the bars are reminders that the calculated flux ratio range is at or above the minimum value. There are 20,200 short horizontal bars, but only a few are shown in Figure 7. The pixel numbers, written above the horizontal axis, indicate which pixels on the x-n plane the horizontal bars correspond to (corresponding ORD\_ and NDX\_ files list, in order from left to right, the indicated flux ratio values and pixel numbers, respectively). The lower half of Figure 7 is analogous to the upper half but represents the maximum calculated values of the same flux ratio.

The measured value of the same flux ratio for one particular particle is indicated in Figure 7 by a horizontal band whose top edge has the flux ratio value (Measurement + Uncertainty) and whose bottom edge is at (Measurement - Uncertainty). This horizontal band is the same in both the minima and maxima halves of the figure. Notice that the bars are calculated values and fixed in place for all time; a different horizontal band is superimposed for each measured particle. Which pixels have an overlap between the measurement band and the calculated ranges? Both plots divide naturally into three regions of answers. In the upper plot, the pixels from the leftmost one out to the marker, A, may or may not overlap, depending on the pixels' maximum values (information not available is in the upper plot). Between markers A and B, the calculated ranges must overlap with the measured range because the minima are embedded in the measured range. Beyond marker B,

no pixels may overlap because the minimum calculated value exceeds the greatest value allowed by measurement.

Similarly, in the lower part of the Figure 7 where calculated maxima are plotted, pixels from No. 1 to marker A cannot overlap, pixels from A to B must overlap, and pixels to the right of marker B might overlap with the measurement band, depending on how low the calculated minima are. A bit of reflection shows that if a pixel is in the "cannot overlap" region of one plot, it must be in the "might overlap" region of the other. Therefore, the aggregate of all the "cannot overlap" pixels from both plots includes, exactly once, every pixel that does not overlap with the measured flux ratio range. The remaining pixels then do overlap (i.e., agree with the measured data for this particular flux ratio). So to find the pixels that do not overlap, we must find point B of the upper plot and point A of the lower plot. More precisely, we must search the file of ordered minimum values to find the number of the first entry that is larger than (Measurement + Uncertainty). For example, if the 12,313th entry were the first entry to exceed (Measurement + Uncertainty), then lines 12,313 through 20,200 of the corresponding NDX\_ file would contain the pixel numbers of pixels, which do not agree with the data. We then search the file of ordered maximum calculated values to find the last entry that is less than (Measurement - Uncertainty) -- perhaps entry number 4002. Then, lines 1 through 4,002 of its corresponding NDX\_ file contain all the remaining pixels that do not satisfy the measurement for this particular flux ratio. The appropriate ranges of the two NDX\_ files can be copied to an array that keeps track of how many times each pixel fails to agree with flux ratio measurements for each particle.

The reason for doing all this is that finding the points A and B is computationally very fast; a simple sequence of binary decisions homes right in on them. For example, to find marker B in the array of minima values, we start at entry No. 10,100 (the midpoint between 1 and 20,200) and ask if the entry value is greater than or less than the target value of (Measurement + Uncertainty). Everything to the left or right of 10,100 (depending on the answer) can be eliminated. We then go to the midpoint of the surviving range and again compare the value found there to the target value, which results in eliminating half that range. After only 15 repetitions ( $2^{15} = 32768 > 20200$ ), we find the desired point in the array. Similarly, 15 comparisons between (Measurement - Uncertainty) and entries in the file of maxima values find the critical point there, point A, and, as a result, the remainder of the nonoverlapping pixels. Thirty yes/no questions asked on the sets of sorted data provide exactly the same information as 20,200 pairs of yes/no questions asked on the original data in a brute force manner.

A separate 20,200 element array accumulates for each pixel the number of times (from 0 to 14) that the calculated and measured flux ratios failed to overlap for each particle. Ideally, only pixels with a score of zero (never failed to overlap) should be counted as solutions for the particle in question. However, because actual measurements of flux ratios may occasionally be in error by more than our best estimate of the experimental uncertainty, it may be desirable to admit solutions that do not necessarily satisfy all 14 of the available measurements. In this investigation, we wanted to see how the number of false returns grew as we pared the number of

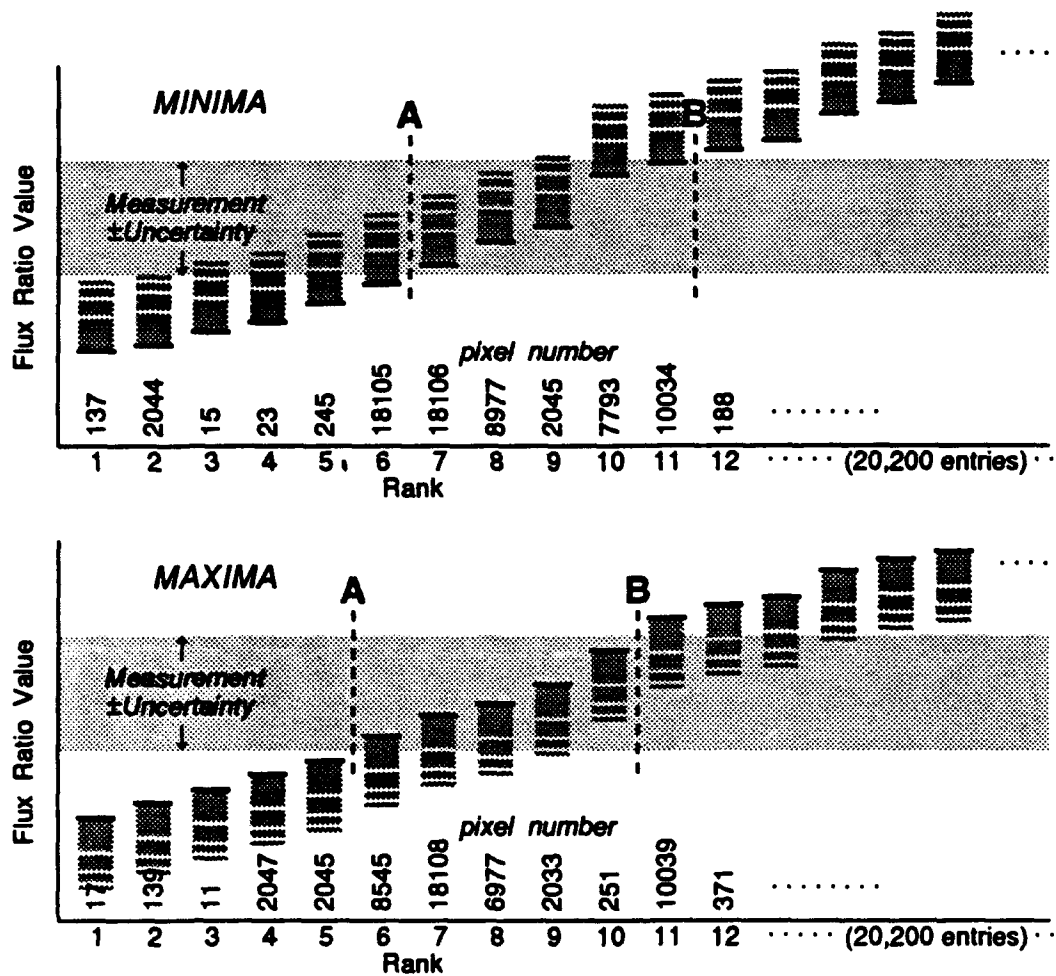


Figure 7. Comparison, for One Flux Ratio, of Calculated (Individual Bars) and Measured (Horizontal Band) Ratio Values

ratios with which agreement was required, and how the domain of solutions varied with different levels of experimental uncertainty. A few of the many tests done are shown in Figures 8-15.

Figures 8-15 are drawn by the page formatting program "PageGarden," by Bloc Publishing Corporation (Coral Gables, FL). The actual output file written by INVERT is a set of statements that instruct PageGarden where to draw pixels in the x-n plane and how dark to shade them, which depends on the number of overlaps. Simple changes to INVERT can alter the information related by the pixel print density.

#### 4.2 Results of the Inversion Trials.

Four pairs of x,n coordinates (indicated by crosses in Figure 8) were selected and used to calculate the four rows of scattering measurements that would be recorded by the SPA instrument sampling the corresponding four spheres. These data were then entered to INVERT and the uncertainty level was set to  $\pm 0.3\%$ . In Figure 8, the solidly shaded pixels are those on which flux ratios formed from the entered as "measured" data agree with previously calculated minimum and maximum flux ratios for all 14 cases. Partially shaded pixels agreed with 12 or 13 of the flux ratio "measurements," and open (nonshaded) pixels agreed with 10 or 11 of the flux ratio "measurements." An uncertainty of only  $0.3\%$  is completely unrealistic. Figure 8 only confirms that INVERT returns the correct solution when given essentially perfect data. However, notice that some spurious returns are already appearing in the upper right of the Figure 8.

Figure 9 shows the return when the stated experimental uncertainty is increased to  $\pm 3.0\%$ . We believe  $3\%$  is about the upper limit for the SPA accuracy; under the most favorable conditions, that accuracy might be approached by one or two of the detectors. There are more returns further from the true solutions, but still the pattern is quite compact.

An accuracy of  $\pm 10\%$  is more typical of the expected SPA performance. This is the uncertainty level assumed in Figure 10, which shows results for the same four spheres. We still see returns that are tightly clustered, except when as few as 10 agreements (overlaps) are accepted.

At  $\pm 30\%$  uncertainty (Figure 11), the number of returns with only 10-11 agreements is becoming quite large. Even worse than the high number of these returns is the way they are distributed in disconnected patches all over the x-n plane; there is no hint of where the right answer might lie. The pattern looks much better for 12-13 agreements and is quite good for 14 agreements. We expect  $30\%$  to be near the lower limit of SPA measurement accuracy.

We have looked at many plots such as those in Figures 8-11, including plots in which the input data was corrupted with random errors, although always within the limits set by the assumed experimental uncertainty. There is surprisingly little difference if the data is actually distorted or not; the nature of the returns is pretty much completely established by the level of experimental uncertainty allowed. Taking  $10\%$  as an average

uncertainty value for the SPA, we concluded that requiring 13 or more agreements of a pixel to return it as a possible inversion solution should produce useful results.

Figures 12 through 15 show the inversion result for 12 spheres, with uncertainty levels of 0.3, 3.0, 10.0, and 30.0% assumed in the measurements. A pixel is shaded if it agrees with at least 13 of the 14 measurements. The outcome is encouraging. We see mostly compact connected patches of returns whose size parameter spread is about 0.3, corresponding to roughly  $0.05 \mu\text{m}$  for blue light. The refractive index spread is not so useful (about 0.1), but the product  $nx$  is very accurately determined for each particle.

## 5. CONCLUSION

We conclude that it is feasible to characterize small dielectric spheres with data measured by the Submicron Particle Analyzer (SPA). The data sets available are not as independent as one could wish for; each additional measurement contributes relatively little to the process of winnowing away unsuitable  $(x,n)$  pairs so that about a dozen measurements are required. Although the method is inefficient, it does apparently work. Matters could be improved by including information not directly related to the flux ratios, such as the number of relative minima in the angular scattering from 0 to  $180^\circ$ . These measurements are suggested by Quist and Wyatt in their paper,<sup>11</sup> which describes an inversion method very similar to this one; however, the SPA does not currently support any types of measurements other than flux ratios.

In the future, we will undertake to demonstrate the inversion method using actual experimental data taken with the SPA. The first step must be an accurate assessment of the instrument's error characteristics as functions of received intensity. If we are successful in the inversion of experimental data, we will attempt to extend the method to spheres of larger size and/or made of absorbing materials. At the same time, we believe improvements can be made to the inversion code itself. It may be possible to replace each of the ordered minimum and maximum calculated flux ratio files with a fairly simple equation that can be solved for the critical points in Figure 7, thereby greatly reducing the size of computer random access memory required to run the inversion program.



TEST CASE: expdat10.tst  
 UNCERTAINTY: +/- 0.3%

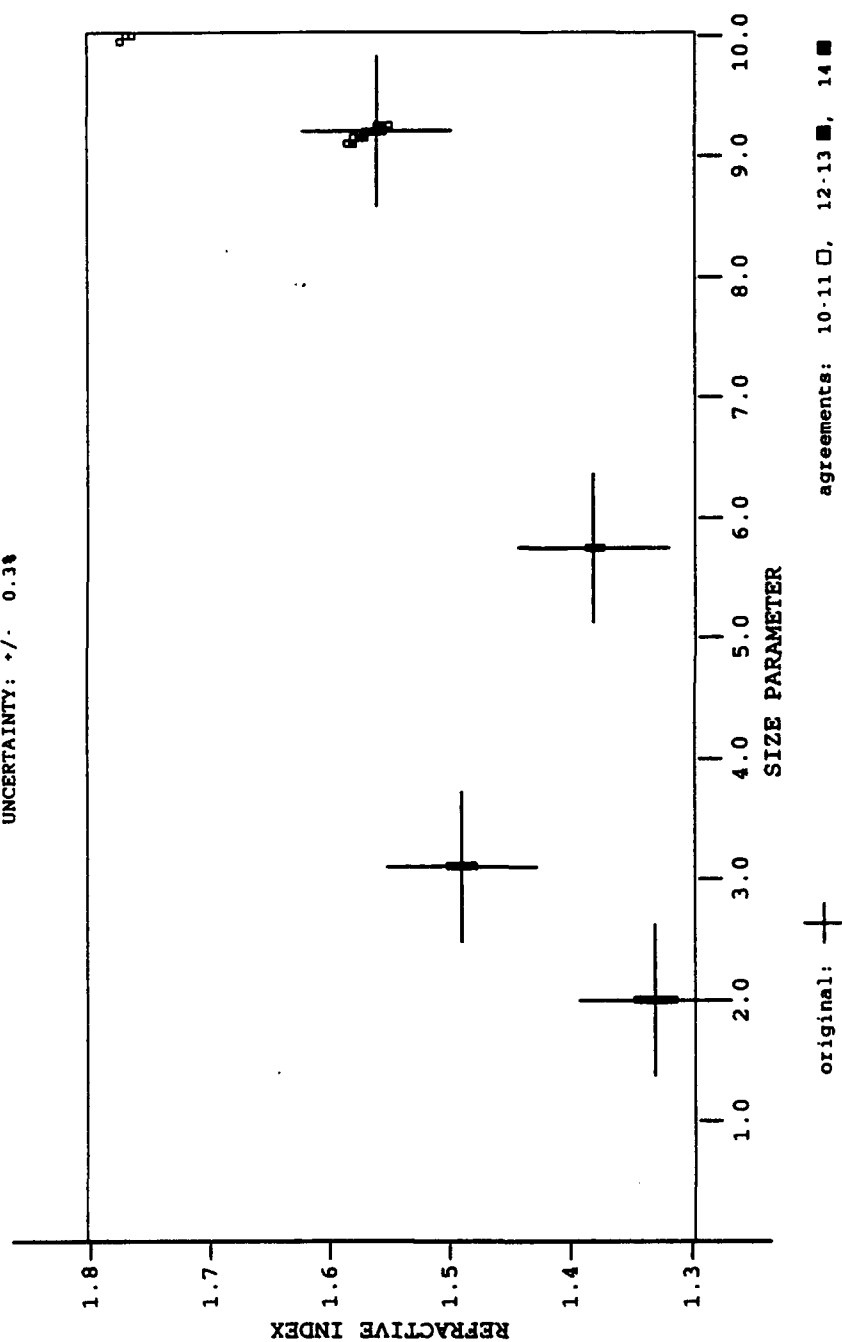


Figure 8. Inversion Results for Four Spheres, Assuming +/- 0.3% Data Uncertainty

TEST CASE: expdat11.tst

UNCERTAINTY:  $\pm 3.0\%$

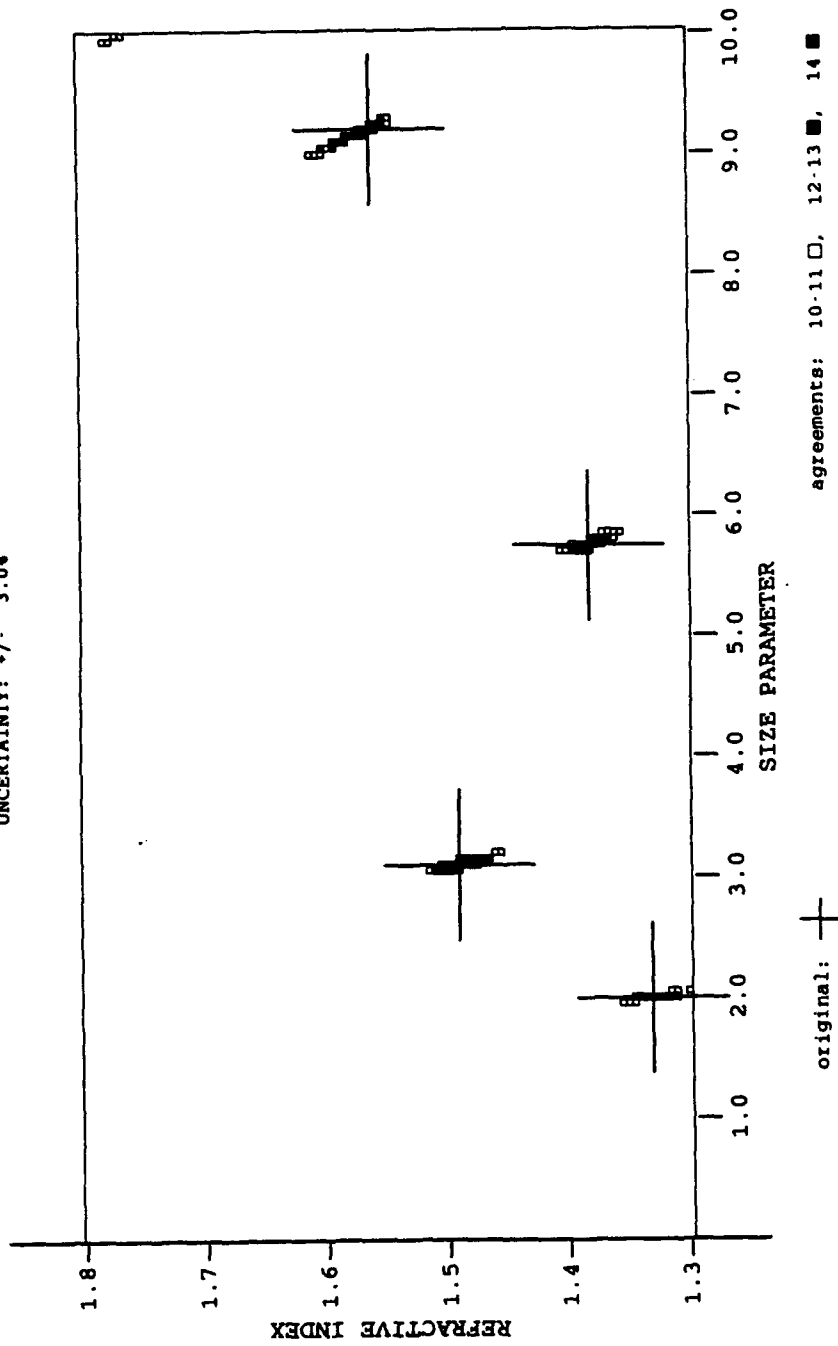


Figure 9. Inversion Results for Four Spheres, Assuming  $\pm 3.0\%$  Data Uncertainty

TEST CASE: exp/at12.tst  
 UNCERTAINTY: +/- 10.0%

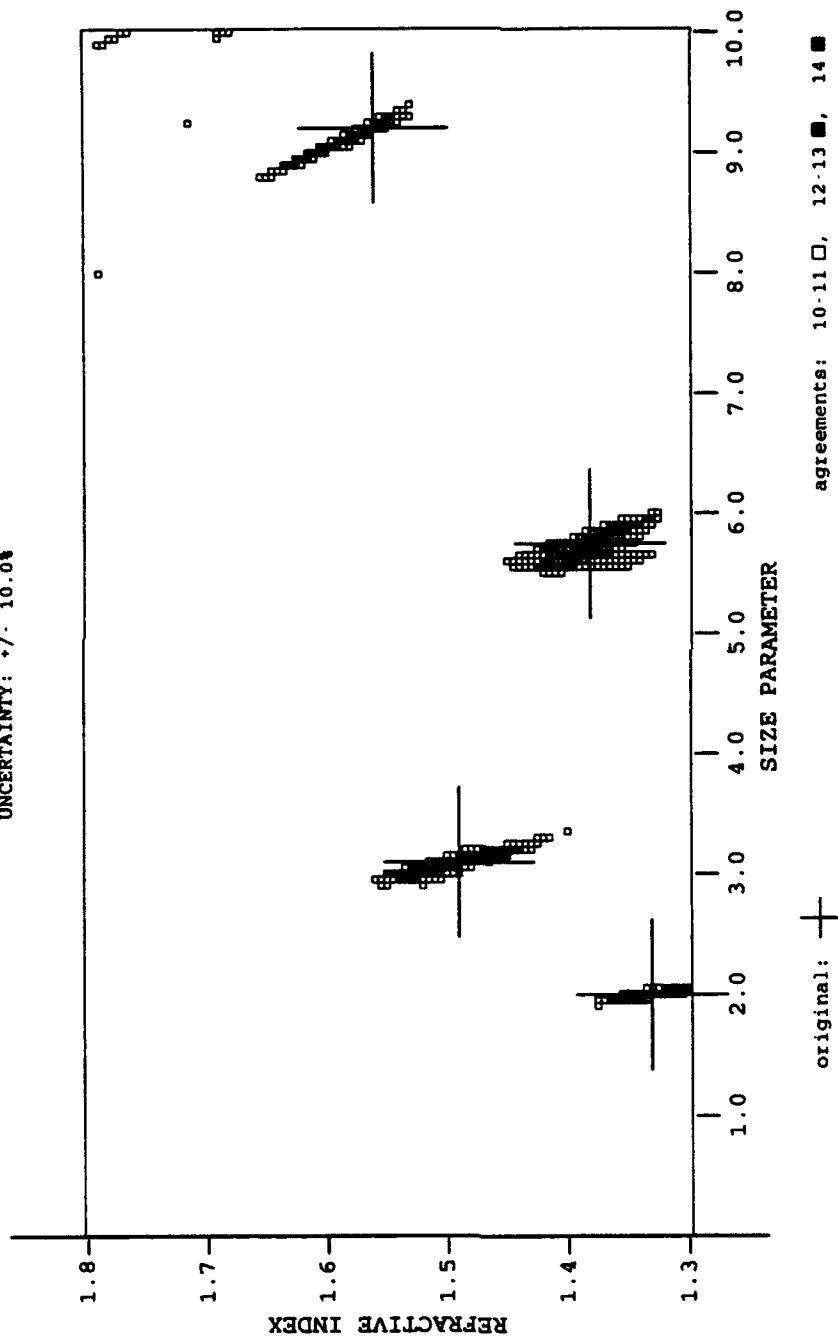


Figure 10. Inversion Results for Four Spheres, Assuming +/- 10.0% Data Uncertainty

TEST CASE: expdat13.tst  
 UNCERTAINTY: +/- 30.0%

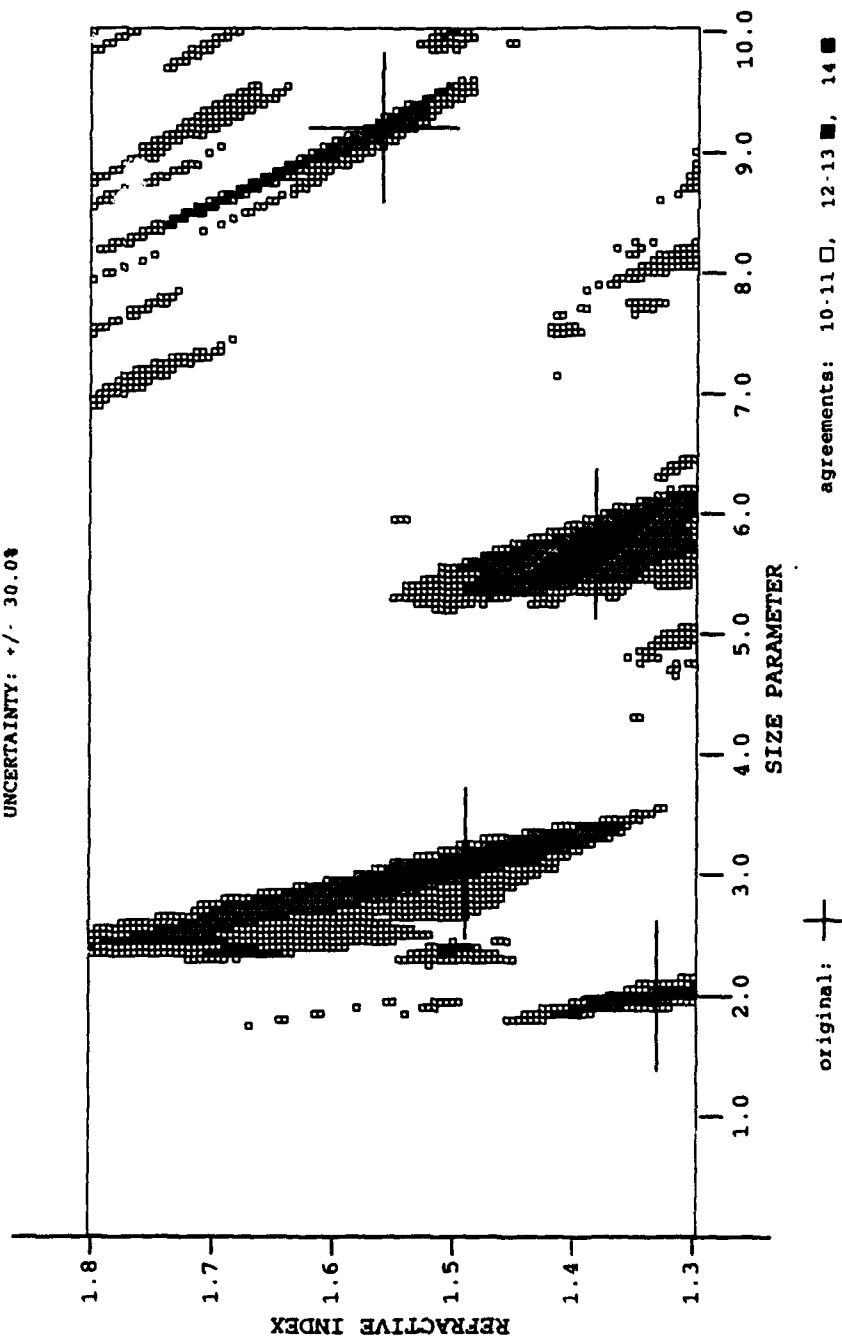


Figure 11. Inversion Results for Twelve Spheres, Assuming +/- 30.0% Data Uncertainty

TEST CASE: expdat50.tst  
 UNCERTAINTY: +/- 0.3%

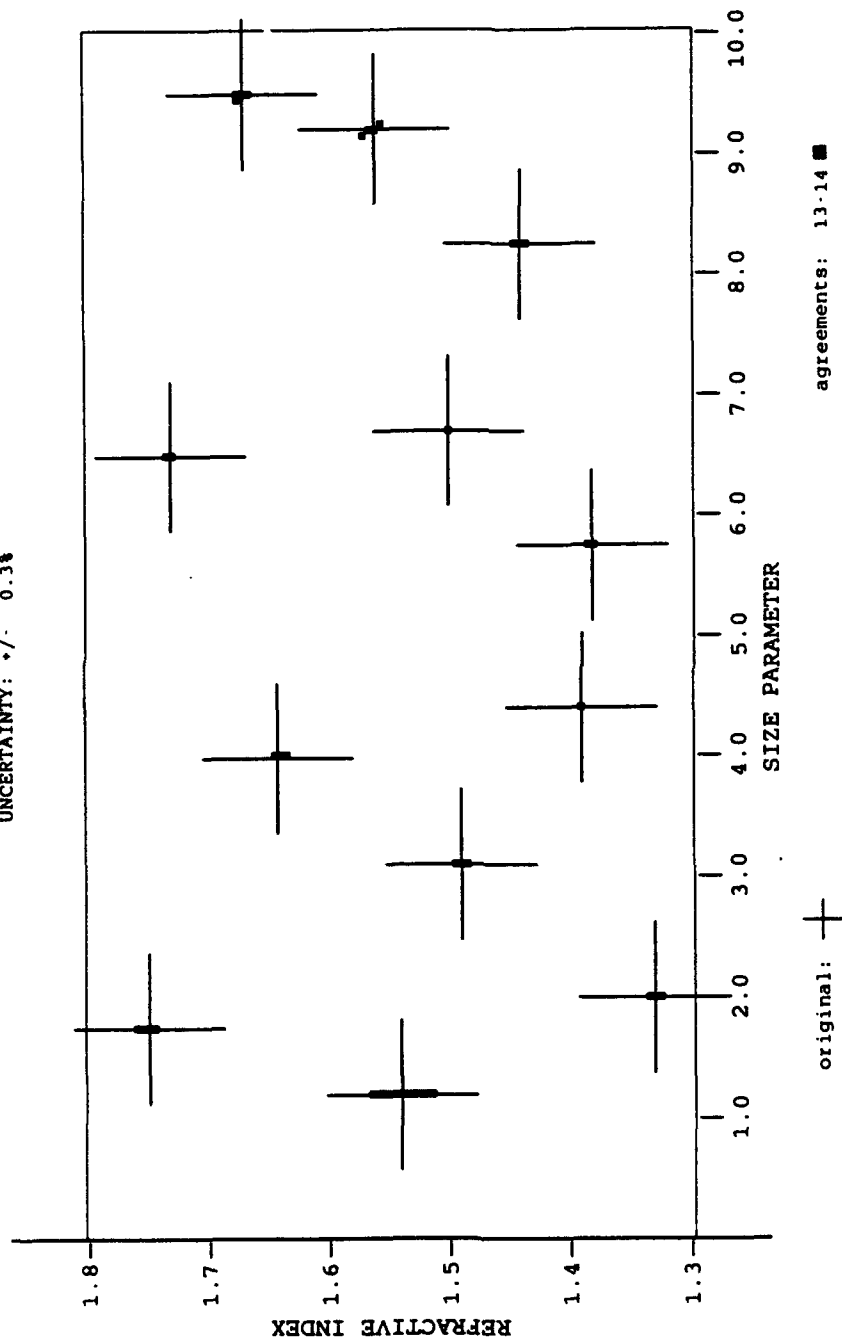


Figure 12. Inversion Results for Twelve Spheres, Assuming +/- 0.3% Data Uncertainty

TEST CASE: expdat51.tst  
 UNCERTAINTY: +/- 3.0%

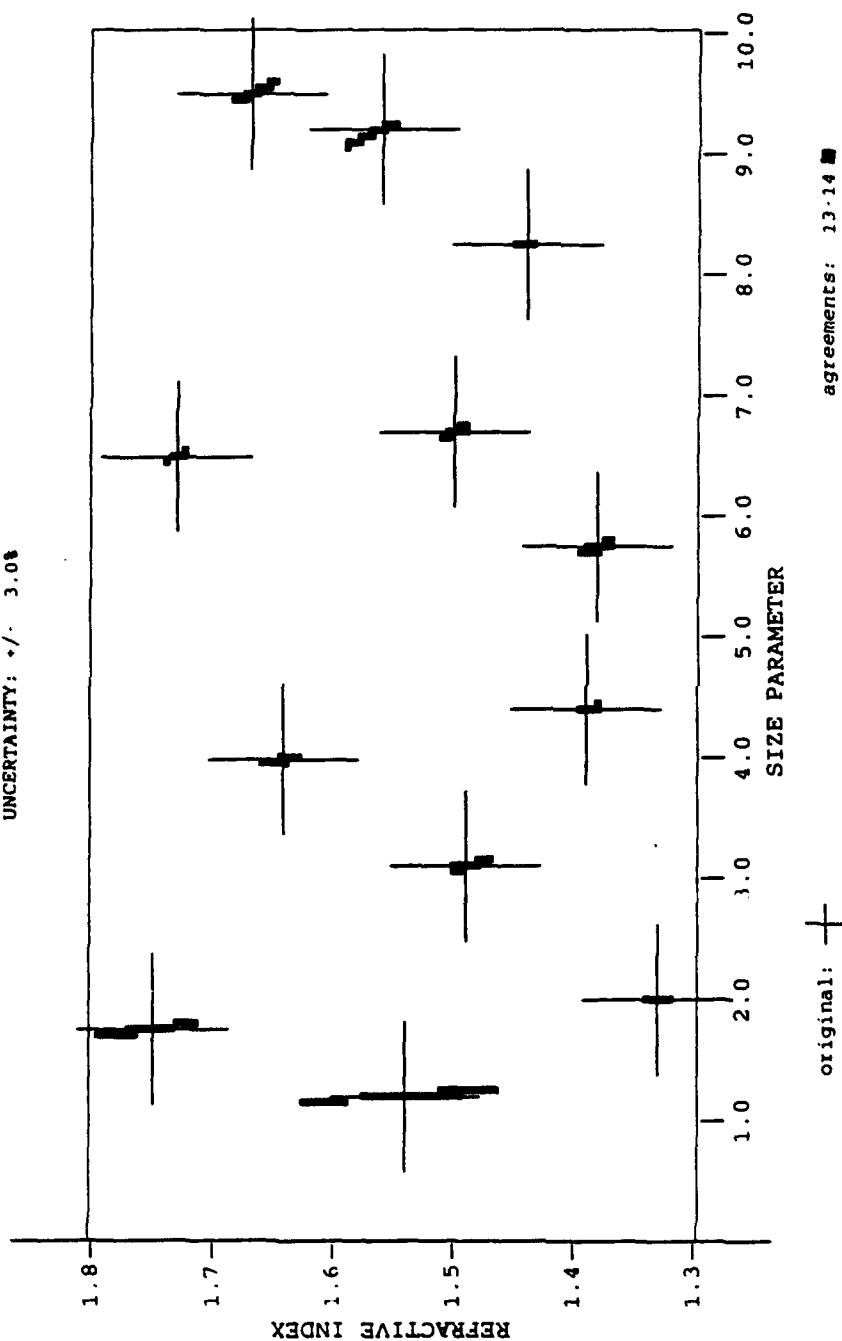


Figure 13. Inversion Results for Twelve Spheres, Assuming +/- 3.0% Data Uncertainty

TEST CASE: expdat52.tst  
 UNCERTAINTY: +/- 10.0%

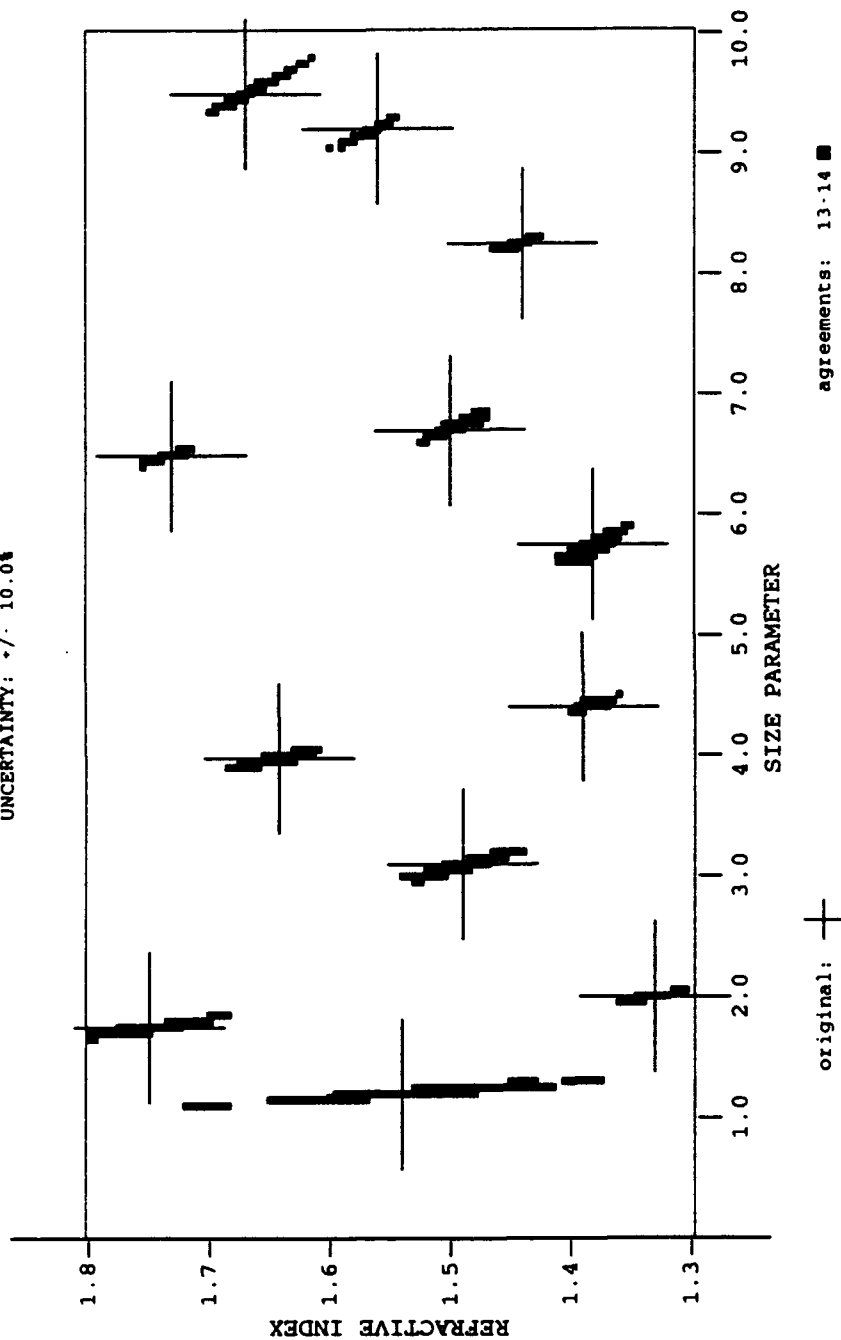


Figure 14. Inversion Results for Twelve Spheres, Assuming +/- 10.0% Data Uncertainty

TEST CASE: expdat53.tst  
 UNCERTAINTY: +/- 30.0%

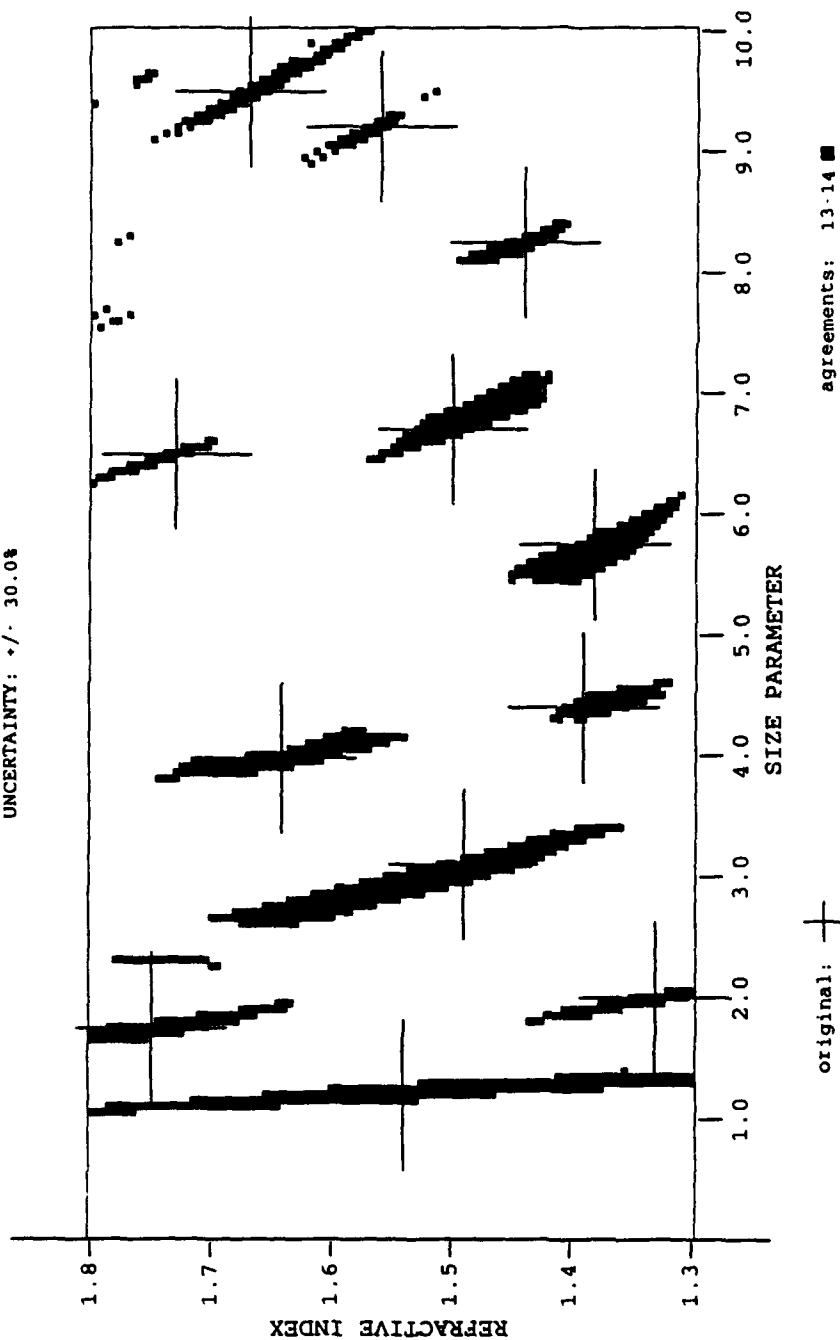


Figure 15. Inversion Results for Twelve Spheres, Assuming +/- 30.0% Data Uncertainty



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APPENDIX A  
HILO.F LISTING

PROGRAM		HILO.F
VERSION		Tue Sep 10 09:18:02 1991
LINE #	SOURCE CODE	PAGE 1
1	PROGRAM HILO	
2 C	NO INPUT DATA. A REGION OF THE X-N PLANE, $0 < X \leq 10$ AND	
3 C	$1.3 \leq N \leq 1.8$ , IS DIVIDED INTO RECTANGLES (PIXELS) WITH DELTA X =	
4 C	.05 AND DELTA N = .005 : 200 COLUMNS AND 101 ROWS. HILO	
5 C	CALCULATES THE MINIMUM AND MAXIMUM VALUES OF EACH OF 27 FLUX	
6 C	RATIOS FOR EACH PIXEL. OUTPUT FILENAMES SPECIFY FLUX NUMERATOR	
7 C	POLARIZATION AND ANGLE; DENOMINATOR ALWAYS U055. ONLY X,N PAIRS	
8 C	ON THE PERIMETERS OF PIXELS CONSIDERED.	
9		
10	INTEGER NROW, NSAMPS, NSQR, DIRECT, K, I	
11	REAL MINMAX(27,2), ACCUM(8,200,27)	
12	CHARACTER*1 DUMMY	
13	CHARACTER FILNAM(54)*8	
14		
15	FILNAM(1) = 'U010.MIN'	
16	FILNAM(2) = 'U010.MAX'	
17	FILNAM(3) = 'H010.MIN'	
18	FILNAM(4) = 'H010.MAX'	
19	FILNAM(5) = 'D010.MIN'	
20	FILNAM(6) = 'D010.MAX'	
21	FILNAM(7) = 'U040.MIN'	
22	FILNAM(8) = 'U040.MAX'	
23	FILNAM(9) = 'H040.MIN'	
24	FILNAM(10) = 'H040.MAX'	
25	FILNAM(11) = 'D040.MIN'	
26	FILNAM(12) = 'D040.MAX'	
27	FILNAM(13) = 'U055.MIN'	
28	FILNAM(14) = 'U055.MAX'	
29	FILNAM(15) = 'H055.MIN'	
30	FILNAM(16) = 'H055.MAX'	
31	FILNAM(17) = 'D055.MIN'	
32	FILNAM(18) = 'D055.MAX'	
33	FILNAM(19) = 'U075.MIN'	
34	FILNAM(20) = 'U075.MAX'	
35	FILNAM(21) = 'H075.MIN'	
36	FILNAM(22) = 'H075.MAX'	
37	FILNAM(23) = 'D075.MIN'	
38	FILNAM(24) = 'D075.MAX'	
39	FILNAM(25) = 'U090.MIN'	
40	FILNAM(26) = 'U090.MAX'	
41	FILNAM(27) = 'H090.MIN'	
42	FILNAM(28) = 'H090.MAX'	
43	FILNAM(29) = 'D090.MIN'	
44	FILNAM(30) = 'D090.MAX'	
45	FILNAM(31) = 'U105.MIN'	
46	FILNAM(32) = 'U105.MAX'	
47	FILNAM(33) = 'H105.MIN'	
48	FILNAM(34) = 'H105.MAX'	
49	FILNAM(35) = 'D105.MIN'	
50	FILNAM(36) = 'D105.MAX'	
51	FILNAM(37) = 'U125.MIN'	
52	FILNAM(38) = 'U125.MAX'	
53	FILNAM(39) = 'H125.MIN'	
54	FILNAM(40) = 'H125.MAX'	
55	FILNAM(41) = 'D125.MIN'	
56	FILNAM(42) = 'D125.MAX'	
57	FILNAM(43) = 'U140.MIN'	
58	FILNAM(44) = 'U140.MAX'	
59	FILNAM(45) = 'H140.MIN'	
60	FILNAM(46) = 'H140.MAX'	

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LINE #	SOURCE CODE	PAGE 2
61	FILNAM(47) = 'D140.MIN'	
62	FILNAM(48) = 'D140.MAX'	
63	FILNAM(49) = 'U170.MIN'	
64	FILNAM(50) = 'U170.MAX'	
65	FILNAM(51) = 'H170.MIN'	
66	FILNAM(52) = 'H170.MAX'	
67	FILNAM(53) = 'D170.MIN'	
68	FILNAM(54) = 'D170.MAX'	
69		
70 C	THE FIRST ROW (N=1.300) AND THE REMAINING 100 ROWS	
71 C	ARE TREATED SEPARATELY	
72		
73 C	***** FIRST ROW *****	
74		
75 C	GET MINS AND MAXS ON ALL FOUR SIDES (DIRECTIONS) OF FIRST SQUARE	
76	NROW = 1	
77	NSQR = 1	
78 C	WHENEVER X < 5, HAVE "SIDE" LOOK AT 6 POINTS ALONG EACH EDGE OF	
79 C	THE PERIMETER	
80	NSAMPS = 6	
81	DO 20 DIRECT=1,4	
82	CALL SIDE(DIRECT, NROW, NSQR, NSAMPS, MINMAX)	
83	DO 22 K=1,27	
84	ACCUM(2*DIRECT-1,NSQR,K) = MINMAX(K,1)	
85	ACCUM(2*DIRECT,NSQR,K) = MINMAX(K,2)	
86	22 CONTINUE	
87	20 CONTINUE	
88		
89 C	REMAINING 199 SQUARES IN THIS FIRST ROW REQUIRE THE CALLING OF	
90 C	"SIDE" FOR EACH OF THREE DIRECTIONS	
91		
92	DO 30 NSQR=2,100	
93 C	WRITE(*,400) NSQR	
94 C 400	FORMAT(1H,'WORKING ON ROW 1 SQUARE ',I3)	
95		
96 C	WEST SIDE OF CURRENT SQUARE = EAST SIDE OF PREVIOUS SQUARE:	
97	DO 32 K=1,27	
98	ACCUM(7,NSQR,K) = ACCUM(3,NSQR-1,K)	
99	ACCUM(8,NSQR,K) = ACCUM(4,NSQR-1,K)	
100	32 CONTINUE	
101	DO 34 DIRECT=1,3	
102	CALL SIDE(DIRECT, NROW, NSQR, NSAMPS, MINMAX)	
103	DO 36 K=1,27	
104	ACCUM(2*DIRECT-1,NSQR,K) = MINMAX(K,1)	
105	ACCUM(2*DIRECT,NSQR,K) = MINMAX(K,2)	
106	36 CONTINUE	
107	34 CONTINUE	
108	30 CONTINUE	
109		
110 C	FOR THE RIGHT HALF OF THE ROW (X>5) INCREASE NSAMPS TO 20	
111 C	AND PROCEED AS BEFORE	
112	NSAMPS = 20	
113		
114	DO 40 NSQR=101,200	
115 C	WRITE(*,401) NSQR	
116 C 401	FORMAT(1H,'WORKING ON ROW 1 SQUARE ',I3)	
117		
118 C	WEST SIDE OF CURRENT SQUARE = EAST SIDE OF PREVIOUS SQUARE:	
119	DO 42 K=1,27	
120	ACCUM(7,NSQR,K) = ACCUM(3,NSQR-1,K)	

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LINE #	SOURCE CODE	PAGE 3
121	ACCUM(8,NSQR,K) = ACCUM(4,NSQR-1,K)	
122	42 CONTINUE	
123	DO 44 DIRECT=1,3	
124	CALL SIDE(DIRECT, NROW, NSQR, NSAMPS, MINMAX)	
125	DO 46 K=1,27	
126	ACCUM(2*DIRECT-1,NSQR,K) = MINMAX(K,1)	
127	ACCUM(2*DIRECT,NSQR,K) = MINMAX(K,2)	
128	46 CONTINUE	
129	44 CONTINUE	
130	40 CONTINUE	
131		
132 C	NOW THE ARRAY ACCUM(8,200,27) IS FILLED WITH DATA FROM THE ENTIRE	
133 C	FIRST ROW. FOR EACH PIXEL IN THE ROW, FIND THE SMALLEST (OF THE	
134 C	FOUR) MINIMUM AND THE LARGEST (OF FOUR) MAXIMUM.	
135 C	OPEN FILES (2 AT A TIME) AND WRITE OUT THE ABSOLUTE MIN AND MAX	
136 C	FLUX RATIOS FOR EACH PIXEL.	
137		
138	DO 50 K=1,27	
139	OPEN(UNIT=3, FILE=FILNAM(2*K-1), ACCESS='SEQUENTIAL',	
140	& FORM='FORMATTED', STATUS='NEW')	
141	OPEN(UNIT=4, FILE=FILNAM(2*K), ACCESS='SEQUENTIAL',	
142	& FORM='FORMATTED', STATUS='NEW')	
143	DO 52 NSQR=1,200	
144	WRITE (3,'(E10.4)') MIN(ACCUM(1,NSQR,K),ACCUM(3,NSQR,K),	
145	& ACCUM(5,NSQR,K),ACCUM(7,NSQR,K))	
146	52 CONTINUE	
147	DO 54 NSQR=1,200	
148	WRITE (4,'(E10.4)') MAX(ACCUM(2,NSQR,K),ACCUM(4,NSQR,K),	
149	& ACCUM(6,NSQR,K),ACCUM(8,NSQR,K))	
150	54 CONTINUE	
151	CLOSE(3)	
152	CLOSE(4)	
153	50 CONTINUE	
154		
155 C	***** THIS ENDS THE FIRST ROW *****	
156 C	*****	
157		
158 C	THE REMAINING 100 ROWS ARE ALL HANDLED THE SAME SO WE HAVE ONE	
159 C	GIANT LOOP FROM HERE TO THE END OF THE PROGRAM:	
160		
161	DO 300 NROW=2,101	
162		
163 C	FOR WHATEVER THE CURRENT ROW IS, PUT THE NORTH MIN AND MAX VALUES	
164 C	OF THE PREVIOUS ROW INTO THE SOUTH MIN AND MAX VALUES OF THE	
165 C	CURRENT ROW FOR EACH OF THE 27 PAGES:	
166		
167	DO 60 K=1,27	
168	DO 62 NSQR=1,200	
169	ACCUM(5,NSQR,K) = ACCUM(1,NSQR,K)	
170	ACCUM(6,NSQR,K) = ACCUM(2,NSQR,K)	
171	62 CONTINUE	
172	60 CONTINUE	
173		
174 C	THE FIRST SQUARE MUST BE TREATED SEPARATELY FROM THE REST:	
175	NSAMPS=6	
176	NSQR=1	
177		
178	CALL SIDE(1,NROW,NSQR,NSAMPS,MINMAX)	
179	DO 70 K=1,27	
180	ACCUM(1,1,K) = MINMAX(K,1)	

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LINE #	SOURCE CODE	PAGE 4
181	ACCUM(2,1,K) = MINMAX(K,2)	
182	70 CONTINUE	
183		
184	CALL SIDE(2,NROW,NSQR,NSAMPS,MINMAX)	
185	DO 72 K=1,27	
186	ACCUM(3,1,K) = MINMAX(K,1)	
187	ACCUM(4,1,K) = MINMAX(K,2)	
188	72 CONTINUE	
189		
190	CALL SIDE(4,NROW,NSQR,NSAMPS,MINMAX)	
191	DO 74 K=1,27	
192	ACCUM(7,1,K) = MINMAX(K,1)	
193	ACCUM(8,1,K) = MINMAX(K,2)	
194	74 CONTINUE	
195		
196 C	THIS COMPLETES THE FIRST SQUARE ONLY. THE REMAINDER OF THE	
197 C	ROW IS DONE IN TWO PARTS; THE LEFT HALF AT LOW RESOLUTION	
198 C	(NSAMPS=6) AND THE RIGHT HALF AT HIGH RESOLUTION (NSAMPS=20):	
199 C	"SIDE" MUST NOW ONLY BE CALLED TWICE FOR EACH PIXEL, SINCE EACH	
200 C	PIXEL'S BOTTOM AND LEFT EDGES HAVE ALREADY BEEN CONSIDERED (AND	
201 C	REMEMBERED IN "ACCUM") AS PARTS OF PREVIOUSLY EVALUATED ADJACENT	
202 C	PIXELS.	
203		
204 C	***** LEFT HALF OF ROW *****	
205		
206	NSAMPS = 6	
207	DO 80 NSQR=2,100	
208		
209 C	WRITE(*,402) NROW, NSQR	
210 C	402 FORMAT(1H ,'WORKING ON ROW ',I3,2X,'SQUARE ',I3)	
211		
212 C	GET CURRENT SQUARE'S WEST SIDE FROM PREVIOUS SQUARE'S EAST SIDE:	
213	DO 82 K=1,27	
214	ACCUM(7,NSQR,K) = ACCUM(3,NSQR-1,K)	
215	ACCUM(8,NSQR,K) = ACCUM(4,NSQR-1,K)	
216	82 CONTINUE	
217		
218	DO 84 DIRECT=1,2	
219	CALL SIDE(DIRECT,NROW,NSQR,NSAMPS,MINMAX)	
220	DO 86 K=1,27	
221	ACCUM(2*DIRECT-1,NSQR,K) = MINMAX(K,1)	
222	ACCUM(2*DIRECT,NSQR,K) = MINMAX(K,2)	
223	86 CONTINUE	
224	84 CONTINUE	
225	80 CONTINUE	
226		
227 C	***** RIGHT HALF OF ROW *****	
228		
229	NSAMPS = 20	
230	DO 90 NSQR=101,200	
231		
232 C	WRITE(*,403) NROW, NSQR	
233 C	403 FORMAT(1H ,'WORKING ON ROW ',I3,2X,'SQUARE ',I3)	
234		
235 C	GET CURRENT SQUARE'S WEST SIDE FROM PREVIOUS SQUARE'S EAST SIDE:	
236	DO 92 K=1,27	
237	ACCUM(7,NSQR,K) = ACCUM(3,NSQR-1,K)	
238	ACCUM(8,NSQR,K) = ACCUM(4,NSQR-1,K)	
239	92 CONTINUE	
240		

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LINE #	SOURCE CODE	PAGE 5
241	DO 94 DIRECT=1,2	
242	CALL SIDE(DIRECT,NROW,NSQR,NSAMPS,MINMAX)	
243	DO 96 K=1,27	
244	ACCUM(2*DIRECT-1,NSQR,K) = MINMAX(K,1)	
245	ACCUM(2*DIRECT,NSQR,K) = MINMAX(K,2)	
246	96 CONTINUE	
247	94 CONTINUE	
248	90 CONTINUE	
249		
250		
251 C	THE 27 PAGES OF ACCUM ARE ALL FILLED NOW FOR THE CURRENT ROW.	
252 C	WRITE RESULTS OUT TO FILES, APPENDING EACH TIME A FILE IS	
253 C	RE-OPENED. (THERE ARE TOO MANY FILES -54- TO HAVE THEM ALL	
254 C	OPENED AT ONCE. WE MUST OPEN AND CLOSE AS NEEDED FOR EACH	
255 C	ROW.) We are still inside the nrow loop	
256		
257	DO 100 K=1,27	
258	OPEN(UNIT=3, FILE=FILNAM(2*K-1), ACCESS='SEQUENTIAL',	
259	& FORM='FORMATTED', STATUS='OLD')	
260	OPEN(UNIT=4, FILE=FILNAM(2*K), ACCESS='SEQUENTIAL',	
261	& FORM='FORMATTED', STATUS='OLD')	
262		
263 C	IN ORDER TO APPEND DATA TO AN 'OLD' FILE, REOPEN FILE AND	
264 C	READ A DUMMY CHARACTER REPEATEDLY TO PLACE THE FILE POINTER TO	
265 C	JUST PAST EOF, THEN BACKSPACE TO 'ERASE' EOF MARKER, LEAVING THE	
266 C	POINTER POINTING TO WHERE EOF USED TO BE. START APPENDING NEW	
267 C	DATA AT THAT LOCATION.	
268		
269	DO 103 I=1,21000	
270	103 READ(3,'(A)',END=105) DUMMY	
271	105 BACKSPACE(3)	
272	DO 102 NSQR=1,200	
273	WRITE (3,'(E10.4)') MIN(ACCUM(1,NSQR,K),ACCUM(3,NSQR,K),	
274	& ACCUM(5,NSQR,K),ACCUM(7,NSQR,K))	
275	102 CONTINUE	
276		
277	DO 107 I=1,21000	
278	107 READ(4,'(A)',END=109) DUMMY	
279	109 BACKSPACE(4)	
280	DO 104 NSQR=1,200	
281	WRITE (4,'(E10.4)') MAX(ACCUM(2,NSQR,K),ACCUM(4,NSQR,K),	
282	& ACCUM(6,NSQR,K),ACCUM(8,NSQR,K))	
283	104 CONTINUE	
284	CLOSE(3)	
285	CLOSE(4)	
286	100 CONTINUE	
287 C	FINISHED APPENDING TO MIN & MAX DATA FILES FOR THIS ROW	
288		
289	300 CONTINUE	
290	STOP	
291	END	
292		
293		
294		
295	SUBROUTINE SIDE (DIRECT, NROW, NSQR, NSAMPS, MINMAX)	
296 C	GIVEN THE LOCATION OF A PIXEL (VIA NROW & NSQR), WHICH OF	
297 C	THE FOUR EDGES TO EVALUALTE (VIA DIRECT), AND THE NUMBER	
298 C	OF EVALUATION POINTS ALONG THAT EDGE (VIA NSAMPS), RETURNS	
299 C	2-D ARRAY MINMAX, WHOSE ROWS CORRESPOND TO THE 27 FLUX RATIOS,	
300 C	AND WHICH GIVES IN COL 1 THE MIN VALUE OF THE FLUX RATIO	

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LINE #	SOURCE CODE	PAGE 6
301	C ALONG GIVEN EDGE AND IN COL 2 THE MAX VALUE.	
302		
303	IMPLICIT DOUBLE PRECISION (A-H,O-Z)	
304	DIMENSION THETD(91), ELTRMX(4,91,2)	
305	INTEGER NROW, NSQR, NSAMPS, SAMP, NDLT, NANG, DIRECT, JX, NM	
306	REAL MINMAX(27,2), IO(28,20), IU, IH, ID	
307		
308	NDLT=1	
309	RFI=0.0	
310	JX=90/NDLT + 1	
311	NANG=0	
312	DO 10 J=1,JX	
313	THETD(J) = DBLE(NANG)	
314	NANG = NANG + NDLT	
315	10 CONTINUE	
316		
317	DELTA = .05/NSAMPS	
318	DELTAN = .005/NSAMPS	
319	CENTRN = 1.300 + .005*(NROW -1)	
320	CENTRX = 0.05 * NSQR	
321		
322	C AT EACH SAMPLING POINT ALONG EDGE, CALC X AND N	
323	DO 20 SAMP=1,NSAMPS	
324	IF (DIRECT .EQ. 1) THEN	
325	RFR = CENTRN + .0025	
326	X = CENTRX -.025 -.5*DELTA + SAMP*DELTA	
327	ELSE IF (DIRECT .EQ. 2) THEN	
328	RFR = CENTRN - .0025 -.5*DELTAN + SAMP*DELTAN	
329	X = CENTRX +.025	
330	ELSE IF (DIRECT .EQ. 3) THEN	
331	RFR = CENTRN - .0025	
332	X = CENTRX -.025 -.5*DELTA + SAMP*DELTA	
333	ELSE IF (DIRECT .EQ. 4) THEN	
334	RFR = CENTRN - .0025 -.5*DELTAN + SAMP*DELTAN	
335	X = CENTRX -.025	
336	ENDIF	
337		
338	C GET SCATT FUNCTIONS VS ANGLE AT SAMPLING POINT, VIA ELTRMX	
339	CALL SMIE (X, RFR, RFI, QSCAT, QEXT, CTBRQS, THETD, ELTRMX, JX)	
340		
341	C FORM UNPOL, HORIZ POL, AND DIAG POL INTENSITIES AT SPA SCATTERING	
342	C ANGLES FROM ELTRMX RETURNS, CORRECTING FOR DETECTOR ACCEPTANCE	
343	C ANGLE. PUT THEM INTO ARRAY IO (27+1 ROWS, ONE FOR EACH FLUX	
344	C RATIO PLUS THE REFERENCE INTENSITY (U055) REPEATED IN LAST ROW),	
345	C AND ONE COL FOR EACH SAMPLING POINT (6 OR 20).	
346	CALL UDHINT(11,1,IU,IH,ID,ELTRMX)	
347	IO(1,SAMP) = IU	
348	IO(2,SAMP) = IH	
349	IO(3,SAMP) = ID	
350		
351	CALL UDHINT(41,1,IU,IH,ID,ELTRMX)	
352	IO(4,SAMP) = IU	
353	IO(5,SAMP) = IH	
354	IO(6,SAMP) = ID	
355		
356	CALL UDHINT(56,1,IU,IH,ID,ELTRMX)	
357	IO(7,SAMP) = IU	
358	IO(8,SAMP) = IH	
359	IO(9,SAMP) = ID	
360		



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LINE #	SOURCE CODE	PAGE 7
361	CALL UDHINT(76,1,IU,IH,ID,ELTRMX)	
362	IO(10,SAMP) = IU	
363	IO(11,SAMP) = IH	
364	IO(12,SAMP) = ID	
365		
366	IU = 0.05825*(ELTRMX(2,90,1)+ELTRMX(1,90,1))	
367	1 +0.3835*(ELTRMX(2,91,1)+ELTRMX(1,91,1))	
368	2 +0.05825*(ELTRMX(2,90,2)+ELTRMX(1,90,2))	
369	IH = 0.05825*ELTRMX(1,90,1)	
370	1 +0.3835*ELTRMX(1,91,1)	
371	2 +0.05825*ELTRMX(1,90,2)	
372	ID = 0.029125*(ELTRMX(2,90,1)+ELTRMX(1,90,1))	
373	1 +0.05825*ELTRMX(4,90,1)	
374	2 +0.19175*(ELTRMX(2,91,1)+ELTRMX(1,91,1))	
375	3 +0.3835*ELTRMX(4,91,1)	
376	4 +0.029125*(ELTRMX(2,90,2)+ELTRMX(1,90,2))	
377	5 +0.05825*ELTRMX(4,90,2)	
378	IO(13,SAMP) = IU	
379	IO(14,SAMP) = IH	
380	IO(15,SAMP) = ID	
381		
382	CALL UDHINT(76,2,IU,IH,ID,ELTRMX)	
383	IO(16,SAMP) = IU	
384	IO(17,SAMP) = IH	
385	IO(18,SAMP) = ID	
386		
387	CALL UDHINT(56,2,IU,IH,ID,ELTRMX)	
388	IO(19,SAMP) = IU	
389	IO(20,SAMP) = IH	
390	IO(21,SAMP) = ID	
391		
392	CALL UDHINT(41,2,IU,IH,ID,ELTRMX)	
393	IO(22,SAMP) = IU	
394	IO(23,SAMP) = IH	
395	IO(24,SAMP) = ID	
396		
397	CALL UDHINT(11,2,IU,IH,ID,ELTRMX)	
398	IO(25,SAMP) = IU	
399	IO(26,SAMP) = IH	
400	IO(27,SAMP) = ID	
401		
402	IO(28,SAMP) = IO(7,SAMP)	
403	20 CONTINUE	
404		
405	C THE ARRAY IO IS NOW FILLED UP WITH INTENSITIES.	
406	C NEXT DIVIDE BY IU055 (IN 28TH ROW) TO GET FLUX RATIOS IN IO	
407		
408	DO 30 IROW=1,27	
409	DO 31 ICOL=1,NSAMPS	
410	IO(IROW,ICOL) = IO(IROW,ICOL) / IO(28,ICOL)	
411	31 CONTINUE	
412	30 CONTINUE	
413		
414	C FILL THE ARRAY MINMAX WITH THE MINIMUM AND MAXIMUM VALUES	
415	C FOR EACH FLUX RATIO	
416		
417	DO 34 K=1,27	
418	MINMAX(K,1) = IO(K,1)	
419	MINMAX(K,2) = IO(K,1)	
420	DO 35 SAMP=2,NSAMPS	

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LINE #	SOURCE CODE	PAGE 8
421	MINMAX(K,1) = MIN(IO(K,SAMP),MINMAX(K,1))	
422	MINMAX(K,2) = MAX(IO(K,SAMP),MINMAX(K,2))	
423	35 CONTINUE	
424		
425	C MINMAX(K,1) NOW CONTAINS THE SMALLEST OF THE NSAMPS VALUES	
426	C OF THE KTH FLUX RATIO	
427	C MINMAX(K,2) NOW CONTAINS THE LARGEST OF THE NSAMPS VALUES	
428	C OF THE KTH FLUX RATIO	
429		
430	34 CONTINUE	
431	RETURN	
432	END	
433		
434		
435		
436	SUBROUTINE SMIE(X,RFR,RFI,QSCAT,QEXT,CTBRQS,THETD,ELTRMX,JX)	
437	C STRAIGHT FROM PETER BARBER'S PROGRAM	
438	C COMMENT C'S ADDED NEAR END TO SUPPRESS PRINTING NO. PARTIAL WAVES	
439	C IMPLICIT DOUBLE PRECISION (A-H,O-Z)	
440	DIMENSION T(4),WFNR(2),WFNI(2),ELTRMX(4,91	
441	1,2),PI(3,91),TAU(3,91),THETD(91),COSTH(91),SINTH2(91)	
442	DIMENSION ACAPR(1050),ACAPI(1050)	
443	DTR = .017453292500	
444	C = RFR**2+RFI**2	
445	RRFR = RFR/C	
446	RRFI = RFI/C	
447	RX = 1.000/X	
448	RRFXR = RRFR*RX	
449	RRFXI = RRFI*RX	
450	NMX2 = IFIX(SNGL(X+4.0500*X**.3333333300+2.000))	
451	IF(NMX2.LE.1050) GO TO 6	
452	WRITE(*,2)	
453	2 FORMAT('KA IS TOO LARGE')	
454	STOP	
455	6 NMX1 = IFIX(SNGL(1.100*X*.0500*(C)))	
456	IF(NMX1.LT.150) NMX1 = 150	
457	CNAR = 0.000	
458	CNAI = 0.000	
459	DO 7 N = NMX1,NMX2,-1	
460	CN = DBLE(FLOAT(N+1))	
461	CNR = CN*RRFXR	
462	CNI = CN*RRFXI	
463	DR = CNR+CNAR	
464	DI = CNI+CNAI	
465	D = DR**2+DI**2	
466	CNAR = CNR-DR/D	
467	CNAI = CNI+DI/D	
468	7 CONTINUE	
469	ACAPR(NMX2) = CNAR	
470	ACAPI(NMX2) = CNAI	
471	NMM = NMX2-1	
472	DO 8 N = NMM,1,-1	
473	CN = DBLE(FLOAT(N+1))	
474	CNR = CN*RRFXR	
475	CNI = CN*RRFXI	
476	DR = CNR+ACAPR(N+1)	
477	DI = CNI+ACAPI(N+1)	
478	D = DR**2+DI**2	
479	ACAPR(N) = CNR-DR/D	
480	ACAPI(N) = CNI+DI/D	

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LINE #	SOURCE CODE	PAGE 9
481	8 CONTINUE	
482	DO 9 J = 1,JX	
483	TH = DTR*THETD(J)	
484	COSTH(J) = DCOS(TH)	
485	SINTH2(J) = DSIN(TH)**2	
486	PI(1,J) = 0.000	
487	PI(2,J) = 1.000	
488	TAU(1,J) = 0.000	
489	TAU(2,J) = COSTH(J)	
490	9 CONTINUE	
491	WM1R = DCOS(X)	
492	WM1I = -DSIN(X)	
493	WFNR(1) = -WM1I	
494	WFNI(1) = WM1R	
495	WFNR(2) = WFNR(1)*RX-WM1R	
496	WFNI(2) = WFNI(1)*RX-WM1I	
497	TC1R = ACAPR(1)*RRFR-ACAPI(1)*RRFI+RX	
498	TC1I = ACAPI(1)*RRFR+ACAPR(1)*RRFI	
499	TC2R = ACAPR(1)*RFR+ACAPI(1)*RFI+RX	
500	TC2I = ACAPI(1)*RFR-ACAPR(1)*RFI	
501	A = TC1R*WFNR(2)-WFNR(1)	
502	B = TC1I*WFNR(2)	
503	C = TC1R*WFNR(2)-TC1I*WFNI(2)-WFNR(1)	
504	D = TC1I*WFNR(2)+TC1R*WFNI(2)-WFNI(1)	
505	CD2 = C**2+D**2	
506	FNAR = (A*C+B*D)/CD2	
507	FNAI = (B*C-A*D)/CD2	
508	A = TC2R*WFNR(2)-WFNR(1)	
509	B = TC2I*WFNR(2)	
510	C = TC2R*WFNR(2)-TC2I*WFNI(2)-WFNR(1)	
511	D = TC2I*WFNR(2)+TC2R*WFNI(2)-WFNI(1)	
512	CD2 = C**2+D**2	
513	FNBR = (A*C+B*D)/CD2	
514	FNBI = (B*C-A*D)/CD2	
515	FNAPR = FNAR	
516	FNAPI = FNAI	
517	FNBPR = FNBR	
518	FNBPI = FNBI	
519	QSCAT = 3.000*(FNAR**2+FNAI**2+FNBR**2+FNBI**2)	
520	QEXT = 3.000*(FNAR+FNBR)	
521	CTBRQS = 0.000	
522	FNAR = 1.500*FNAR	
523	FNAI = 1.500*FNAI	
524	FNBR = 1.500*FNBR	
525	FNBI = 1.500*FNBI	
526	DO 10 J = 1,JX	
527	ELTRMX(1,J,1) = FNAR*PI(2,J)+FNBR*TAU(2,J)	
528	ELTRMX(2,J,1) = FNAI*PI(2,J)+FNBI*TAU(2,J)	
529	ELTRMX(3,J,1) = FNBR*PI(2,J)+FNAR*TAU(2,J)	
530	ELTRMX(4,J,1) = FNBI*PI(2,J)+FNAI*TAU(2,J)	
531	ELTRMX(1,J,2) = FNAR*PI(2,J)-FNBR*TAU(2,J)	
532	ELTRMX(2,J,2) = FNAI*PI(2,J)-FNBI*TAU(2,J)	
533	ELTRMX(3,J,2) = FNBR*PI(2,J)-FNAR*TAU(2,J)	
534	ELTRMX(4,J,2) = FNBI*PI(2,J)-FNAI*TAU(2,J)	
535	10 CONTINUE	
536	N = 2	
537	DO 15 I = 1,NMX2	
538	FN = DBLE(FLOAT(N))	
539	T(1) = 2.000*FN-1.000	
540	T(2) = FN-1.000	

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LINE #	SOURCE CODE	PAGE 10
541	T(3) = 2.000*FN+1.000	
542	DO 11 J = 1,JX	
543	PI(3,J) = (T(1)*PI(2,J)*COSTH(J)-FN*PI(1,J))/T(2)	
544	TAU(3,J) = COSTH(J)*(PI(3,J)-PI(1,J))-T(1)*SINTH2(J)*PI(2,J)+TAU(1	
545	1,J)	
546	11 CONTINUE	
547	WM1R = WFNR(1)	
548	WM1I = WFNI(1)	
549	WFNR(1) = WFNR(2)	
550	WFNI(1) = WFNI(2)	
551	WFNR(2) = T(1)*RX*WFNR(1)-WM1R	
552	WFNI(2) = T(1)*RX*WFNI(1)-WM1I	
553	TC1R = ACAPR(N)*RRFR-ACAPI(N)*RRFI+FN*RX	
554	TC1I = ACAPE(N)*RRFR+ACAPR(N)*RRFI	
555	TC2R = ACAPR(N)*RFR+ACAPI(N)*RFI+FN*RX	
556	TC2I = ACAPE(N)*RFR-ACAPR(N)*RFI	
557	A = TC1R*WFNR(2)-WFNR(1)	
558	B = TC1I*WFNR(2)	
559	C = TC1R*WFNR(2)-TC1I*WFNI(2)-WFNR(1)	
560	D = TC1I*WFNR(2)+TC1R*WFNI(2)-WFNI(1)	
561	CD2 = C**2+D**2	
562	FNAR = (A*C+B*D)/CD2	
563	FNAI = (B*C-A*D)/CD2	
564	A = TC2R*WFNR(2)-WFNR(1)	
565	B = TC2I*WFNR(2)	
566	C = TC2R*WFNR(2)-TC2I*WFNI(2)-WFNR(1)	
567	D = TC2I*WFNR(2)+TC2R*WFNI(2)-WFNI(1)	
568	CD2 = C**2+D**2	
569	FNBR = (A*C+B*D)/CD2	
570	FNBI = (B*C-A*D)/CD2	
571	T(4) = T(1)/(FN*T(2))	
572	T(2) = (T(2)*(FN+1.000))/FN	
573	CTBRQS = CTBRQS+T(2)*(FNAPR*FNAR+FNAPI*FNAI+FNBRP*FNBR+FNBP*FNBI)	
574	1+T(4)*(FNAPR*FNBRP+FNAPI*FNBP)	
575	T(4) = FNAR**2+FNAI**2+FNBR**2+FNBI**2	
576	QSCAT = QSCAT+T(3)*T(4)	
577	QEXT = QEXT+T(3)*(FNAR+FNBR)	
578	T(2) = FN*(FN+1.000)	
579	T(1) = T(3)/T(2)	
580	K = (N/2)*2	
581	DO 13 J = 1,JX	
582	ELTRMX(1,J,1) = ELTRMX(1,J,1)+T(1)*(FNAR*PI(3,J)+FNBR*TAU(3,J))	
583	ELTRMX(2,J,1) = ELTRMX(2,J,1)+T(1)*(FNAI*PI(3,J)+FNBI*TAU(3,J))	
584	ELTRMX(3,J,1) = ELTRMX(3,J,1)+T(1)*(FNBR*PI(3,J)+FNAR*TAU(3,J))	
585	ELTRMX(4,J,1) = ELTRMX(4,J,1)+T(1)*(FNBI*PI(3,J)+FNAI*TAU(3,J))	
586	IF(K.EQ.N) GO TO 12	
587	ELTRMX(1,J,2) = ELTRMX(1,J,2)+T(1)*(FNAR*PI(3,J)-FNBR*TAU(3,J))	
588	ELTRMX(2,J,2) = ELTRMX(2,J,2)+T(1)*(FNAI*PI(3,J)-FNBI*TAU(3,J))	
589	ELTRMX(3,J,2) = ELTRMX(3,J,2)+T(1)*(FNBR*PI(3,J)-FNAR*TAU(3,J))	
590	ELTRMX(4,J,2) = ELTRMX(4,J,2)+T(1)*(FNBI*PI(3,J)-FNAI*TAU(3,J))	
591	GO TO 13	
592	12 ELTRMX(1,J,2) = ELTRMX(1,J,2)+T(1)*(-FNAR*PI(3,J)+FNBR*TAU(3,J))	
593	ELTRMX(2,J,2) = ELTRMX(2,J,2)+T(1)*(-FNAI*PI(3,J)+FNBI*TAU(3,J))	
594	ELTRMX(3,J,2) = ELTRMX(3,J,2)+T(1)*(-FNBR*PI(3,J)+FNAR*TAU(3,J))	
595	ELTRMX(4,J,2) = ELTRMX(4,J,2)+T(1)*(-FNBI*PI(3,J)+FNAI*TAU(3,J))	
596	13 CONTINUE	
597	IF(T(4).LT.1.00-14) GO TO 20	
598	N = N+1	
599	DO 14 J = 1,JX	
600	PI(1,J) = PI(2,J)	

PROGRAM

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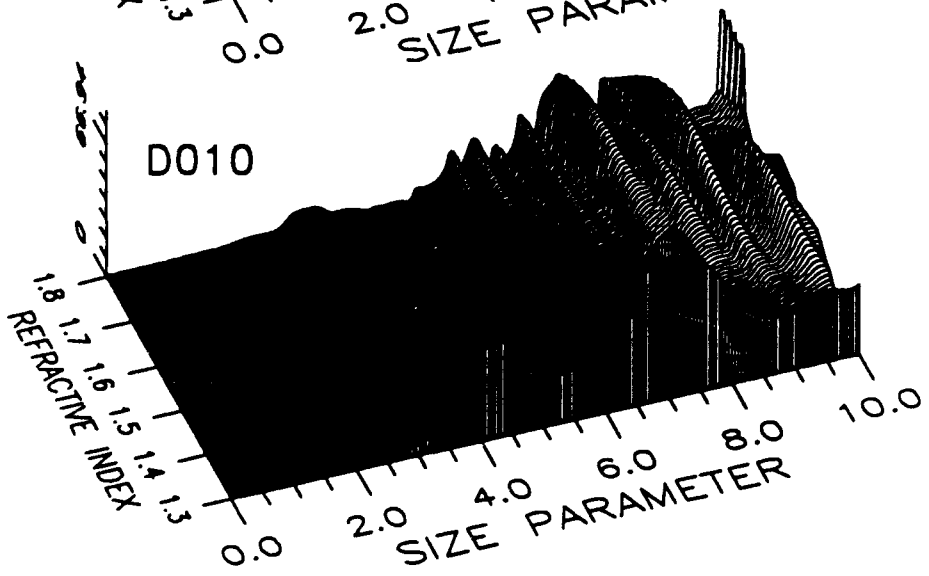
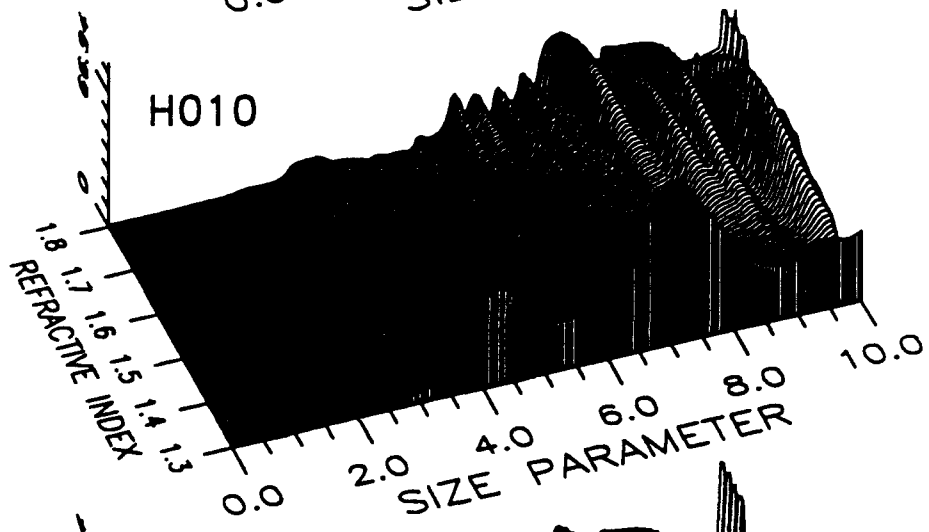
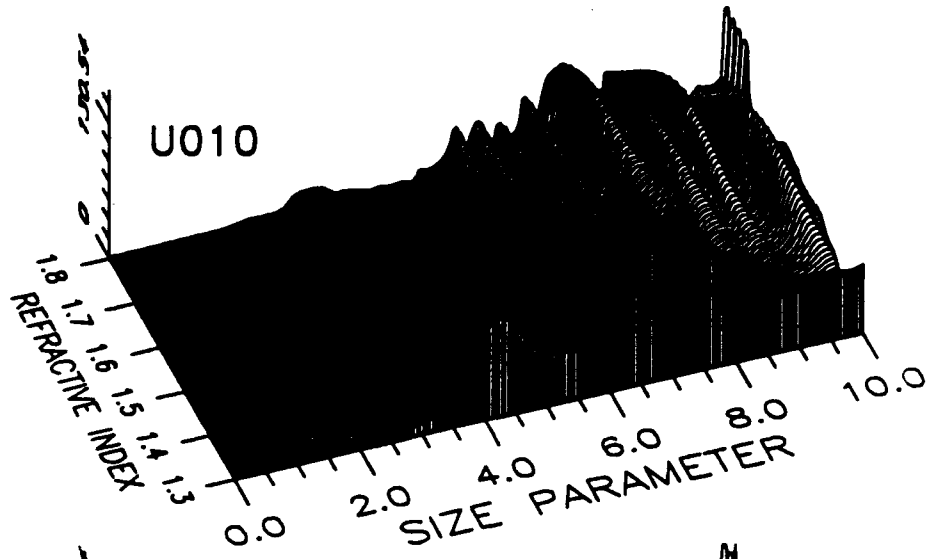
VERSION

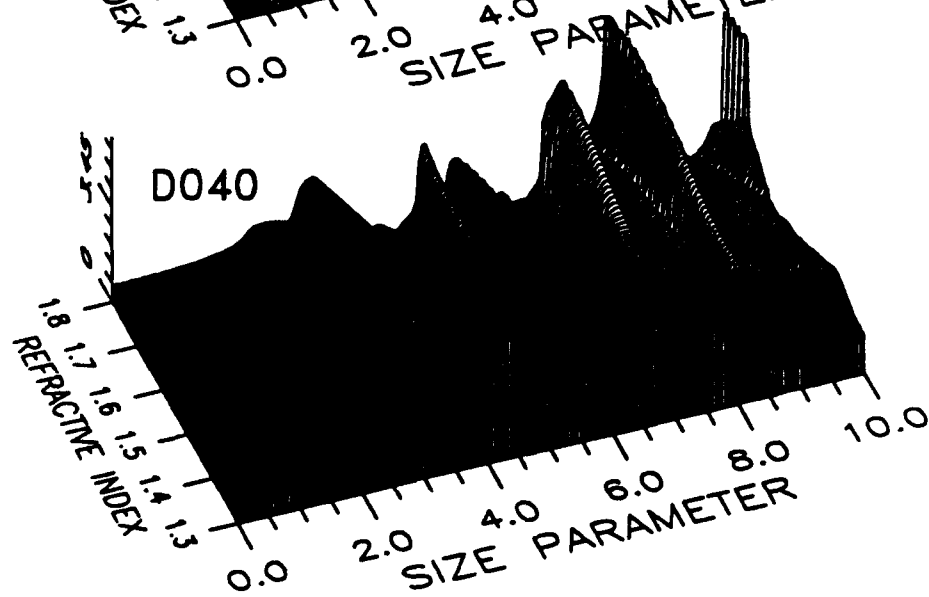
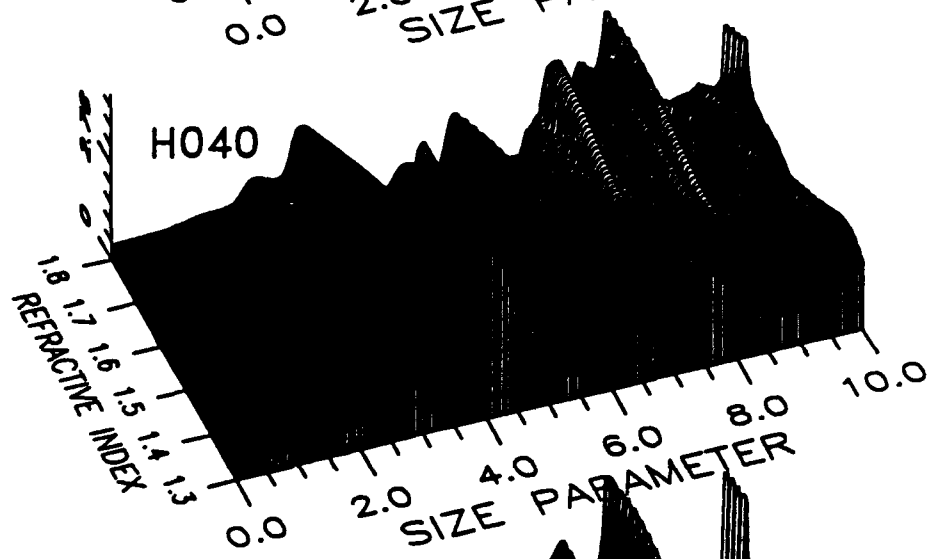
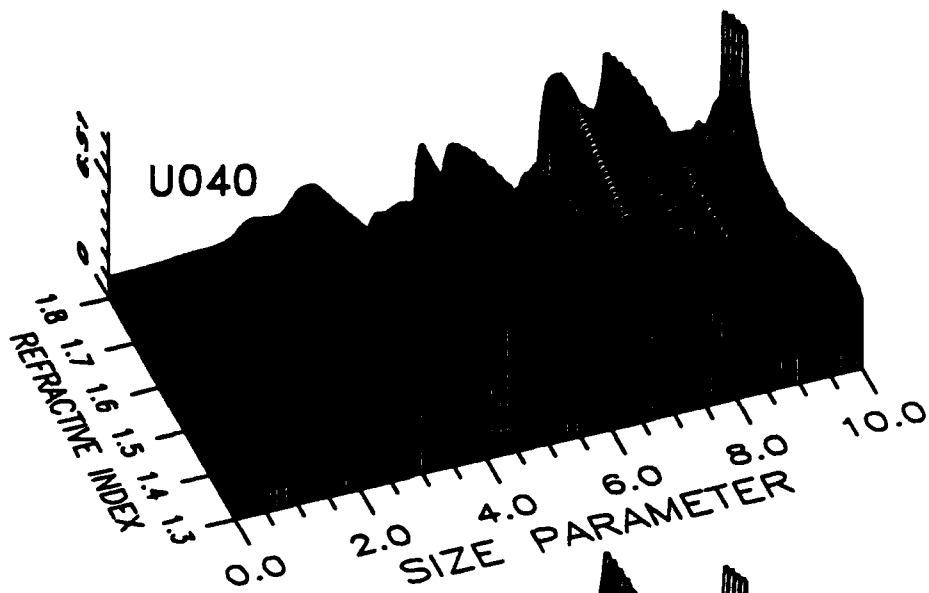
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LINE #	SOURCE CODE	PAGE 11
601	PI(2,J) = PI(3,J)	
602	TAU(1,J) = TAU(2,J)	
603	TAU(2,J) = TAU(3,J)	
604	14 CONTINUE	
605	FNAPR = FNAR	
606	FNAPI = FNAI	
607	FNBPR = FNBR	
608	FNBPI = FNBI	
609	15 CONTINUE	
610	QSCAT = 0.000	
611	QEXT = 0.000	
612	RETURN	
613	20 DO 30 J = 1,JX	
614	DO 30 K = 1,2	
615	DO 25 I = 1,4	
616	T(I) = ELTRMX(I,J,K)	
617	25 CONTINUE	
618	ELTRMX(2,J,K) = T(1)**2+T(2)**2	
619	ELTRMX(1,J,K) = T(3)**2+T(4)**2	
620	ELTRMX(3,J,K) = T(1)*T(3)+T(2)*T(4)	
621	ELTRMX(4,J,K) = T(2)*T(3)-T(4)*T(1)	
622	30 CONTINUE	
623	C = 2.000*RX**2	
624	QSCAT = C*QSCAT	
625	QEXT = C*QEXT	
626	CTBRQS = 2.000*CTBRQS*C	
627	C WRITE(6,200) N	
628	C 200 FORMAT(I6)	
629	RETURN	
630	END	
631		
632	SUBROUTINE UDHINT(JJ, KK, IU, IH, ID, ELTRMX)	
633	C GIVEN INTEGERS WHICH TOGETHER SPECIFY A PARTICULAR ONE OF THE	
634	C NINE SPA SCATTERING ANGLES (JJ & KK), AND THE COMPLETE ARRAY	
635	C ELTRMX, RETURNS COMBINATIONS OF THE SCATTERING MATRIX ELEMENTS	
636	C FOR THE GIVEN ANGLE, WITH CORRECTION FOR FINITE DETECTOR	
637	C ACCEPTANCE ANGLE ACCOMPLISHED BY ADDING IN BITS FROM SCATTERING	
638	C ANGLES ONE DEGREE HIGHER AND LOWER.	
639	REAL IU, IH, ID	
640	INTEGER JJ, KK	
641	DOUBLE PRECISION ELTRMX(4,91,2)	
642		
643	IU = 0.05825*(ELTRMX(2, JJ-1, KK)+ELTRMX(1, JJ-1, KK))	
644	1 +0.3835*(ELTRMX(2, JJ, KK)+ELTRMX(1, JJ, KK))	
645	2 +0.05825*(ELTRMX(2, JJ+1, KK)+ELTRMX(1, JJ+1, KK))	
646	IH = 0.05825*ELTRMX(1, JJ-1, KK)	
647	1 +0.3835*ELTRMX(1, JJ, KK)	
648	2 +0.05825*ELTRMX(1, JJ+1, KK)	
649	ID = 0.029125*(ELTRMX(2, JJ-1, KK)+ELTRMX(1, JJ-1, KK))	
650	1 +0.05825*ELTRMX(4, JJ-1, KK)	
651	2 +0.19175*(ELTRMX(2, JJ, KK)+ELTRMX(1, JJ, KK))	
652	3 +0.3835*ELTRMX(4, JJ, KK)	
653	4 +0.029125*(ELTRMX(2, JJ+1, KK)+ELTRMX(1, JJ+1, KK))	
654	5 +0.05825*ELTRMX(4, JJ+1, KK)	
655		
656	RETURN	
657	END	

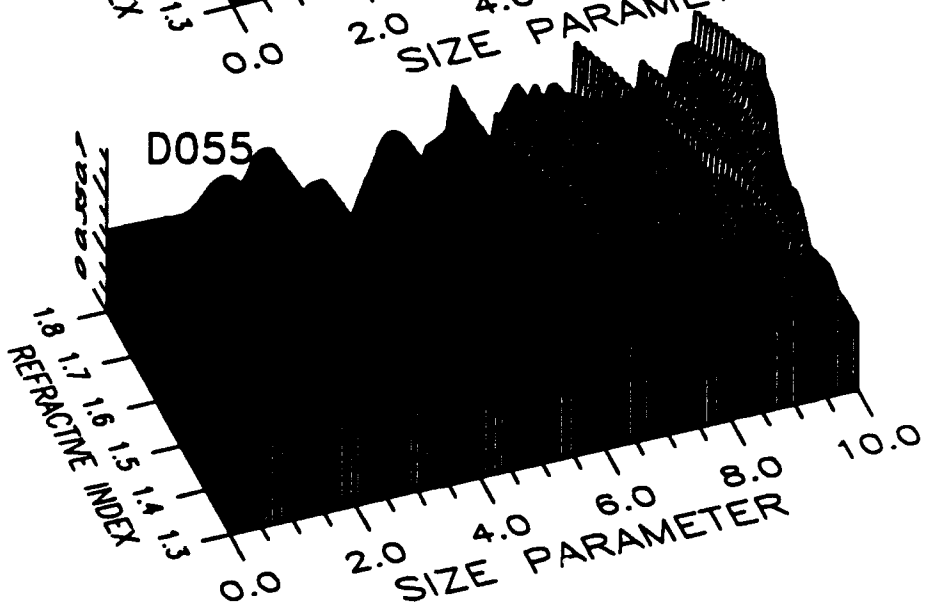
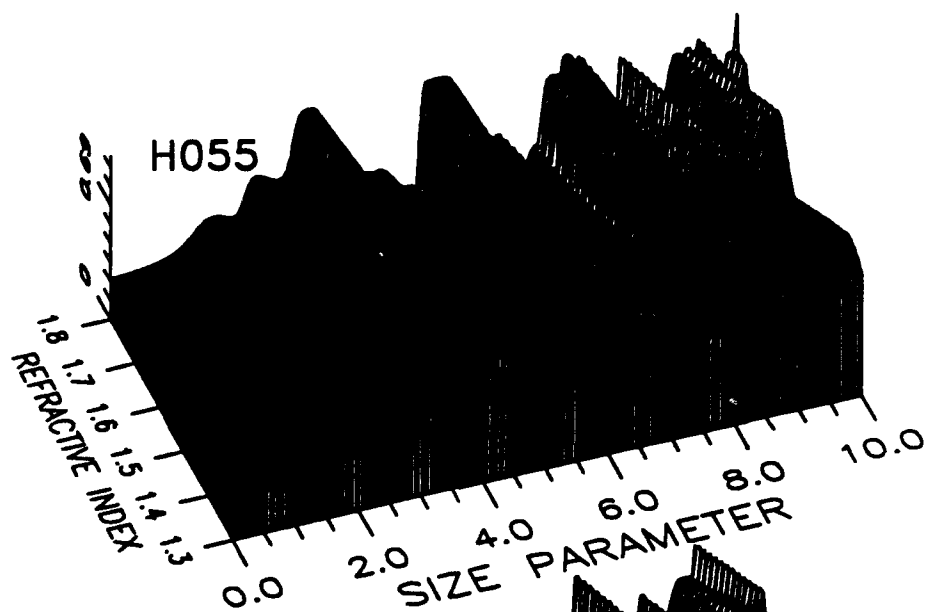
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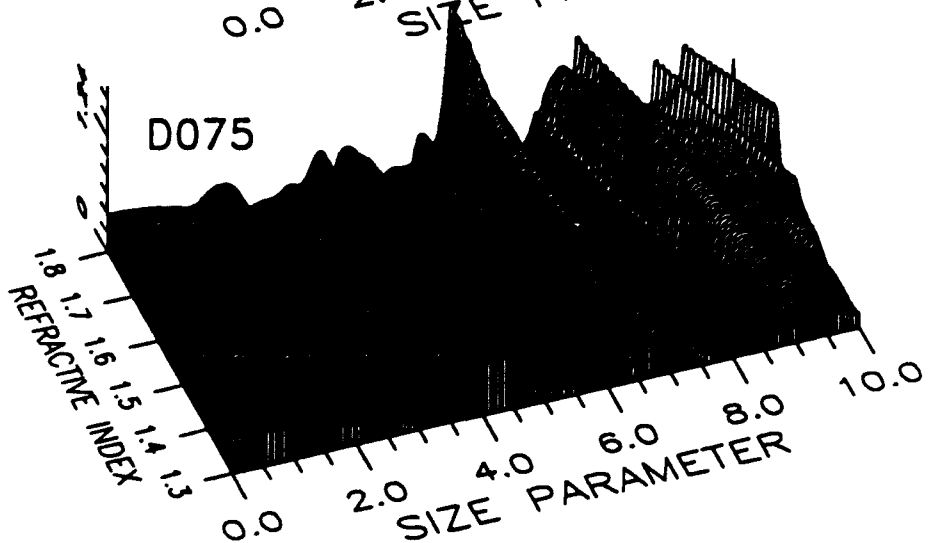
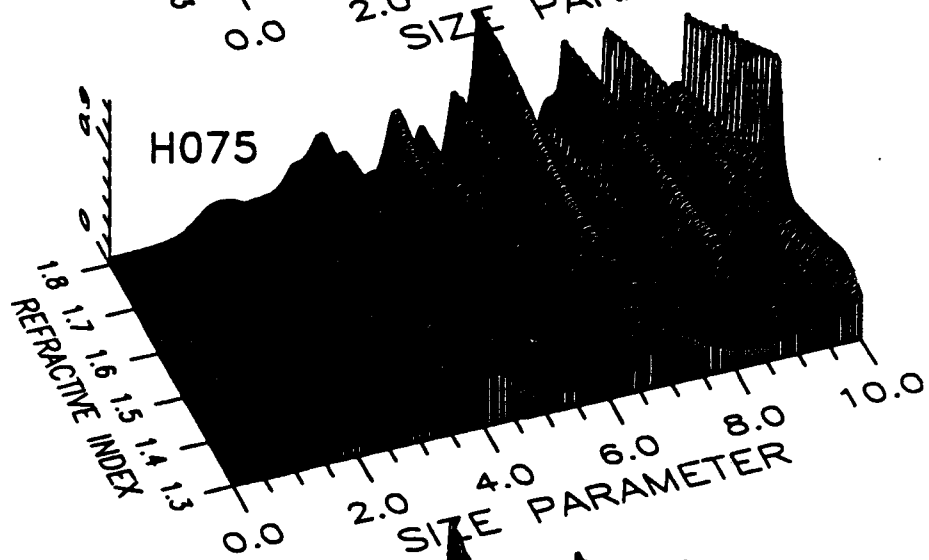
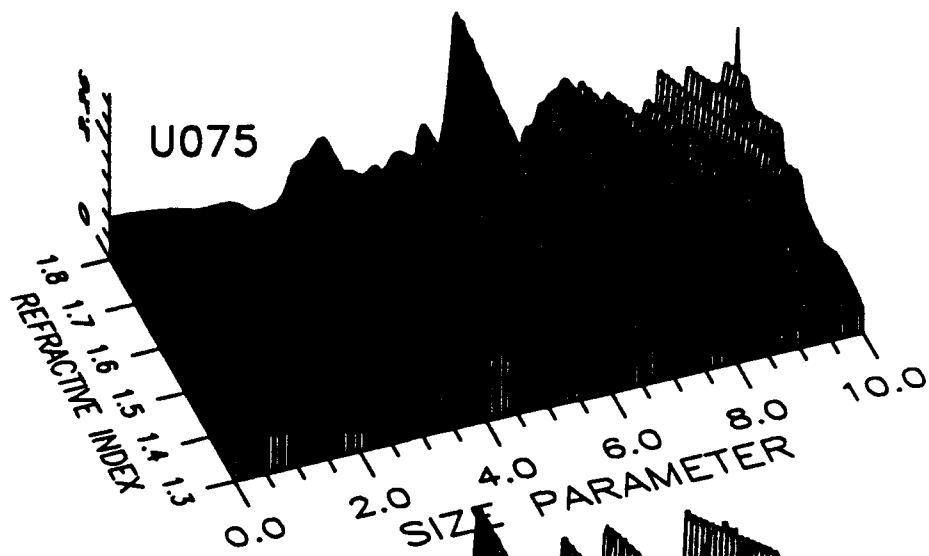
APPENDIX B  
CALCULATED RATIO MAPS

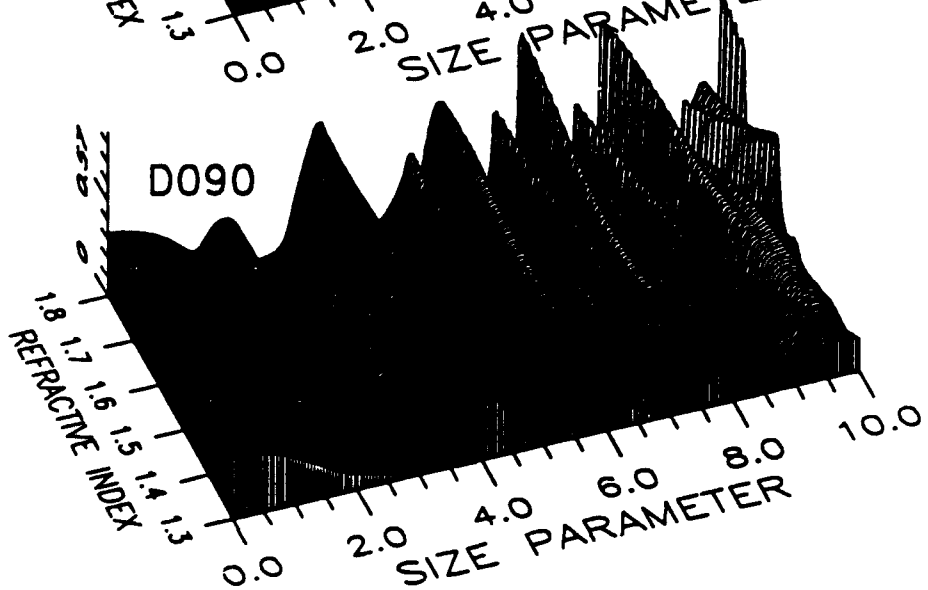
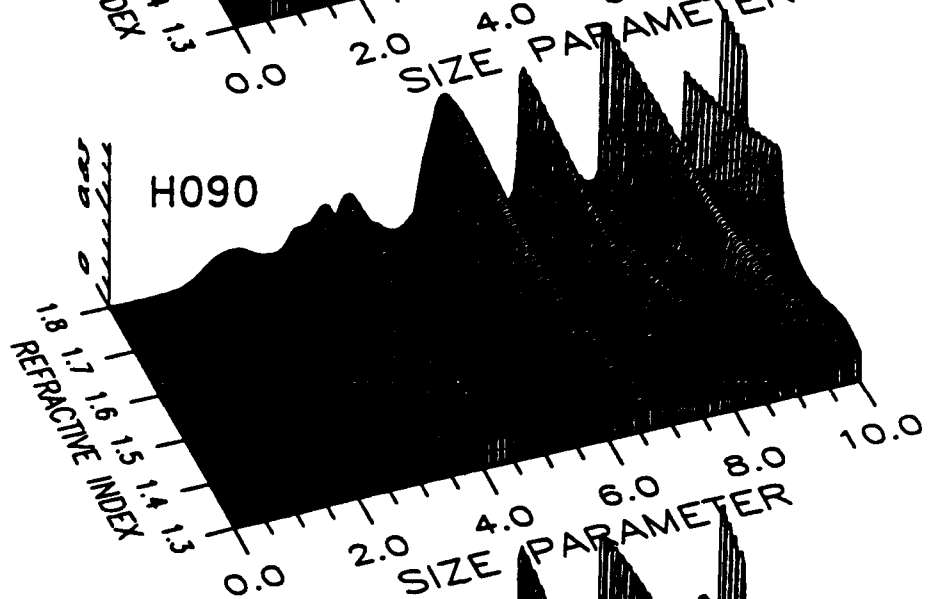
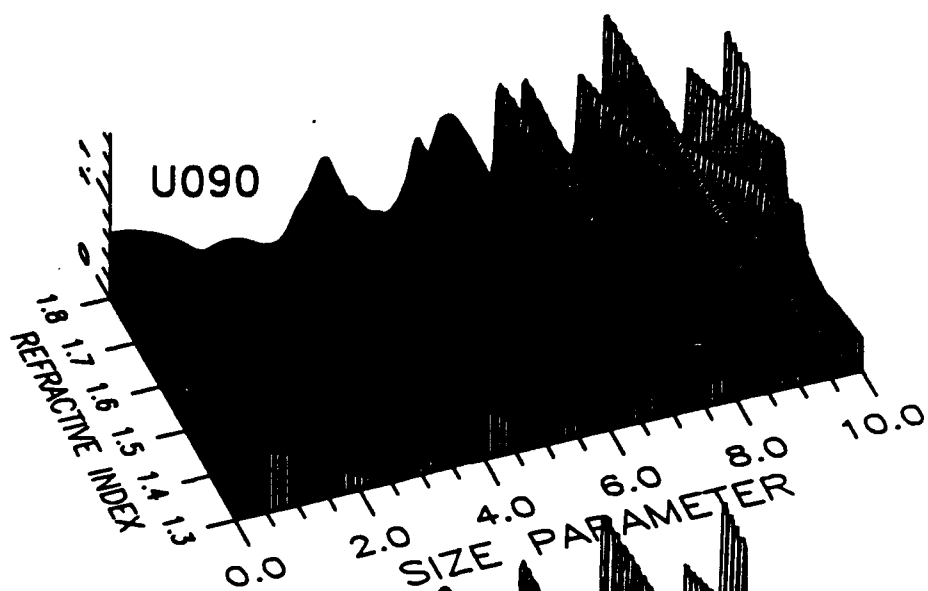


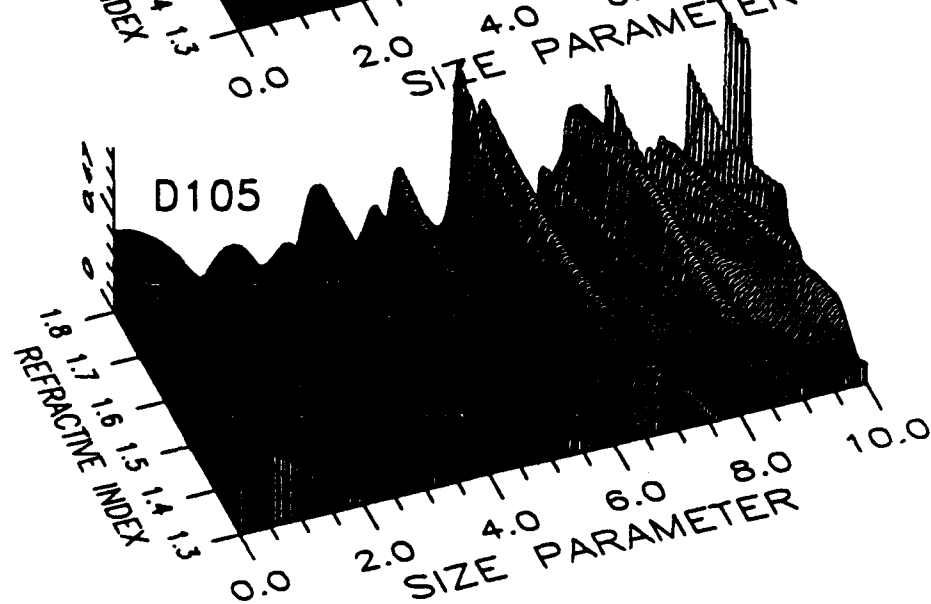
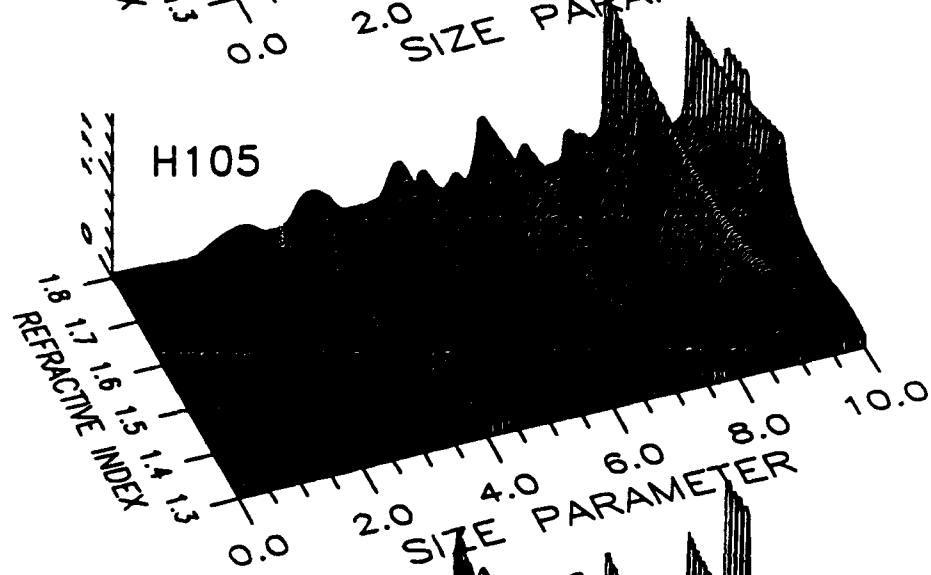
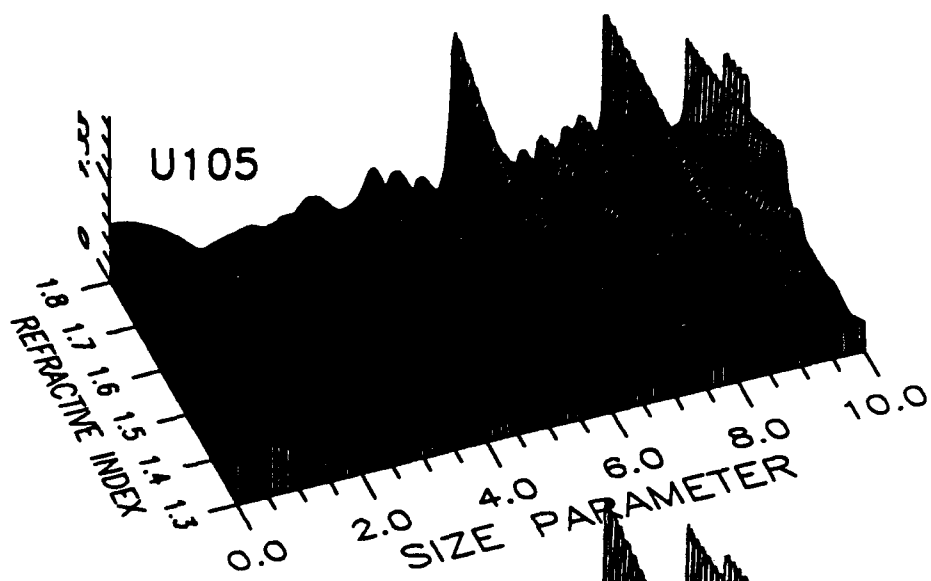


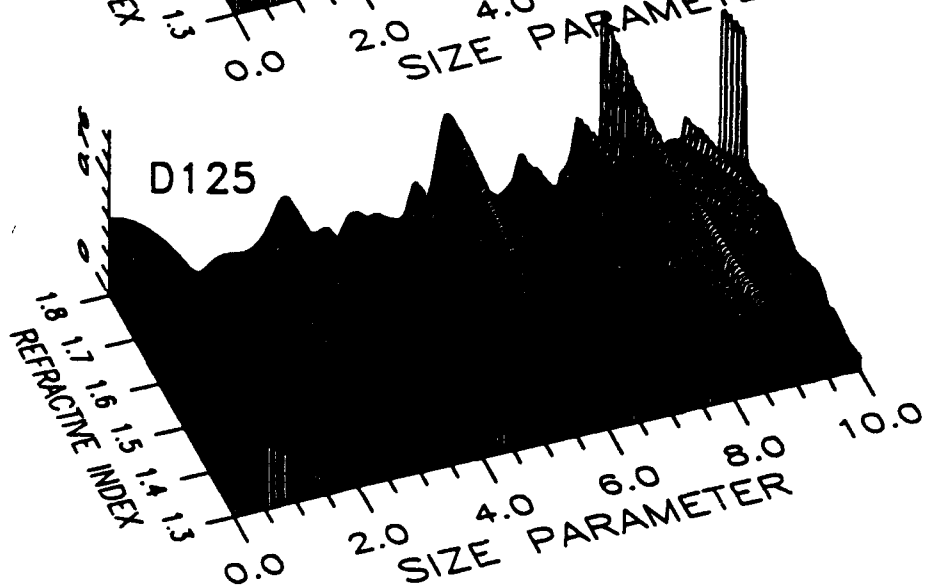
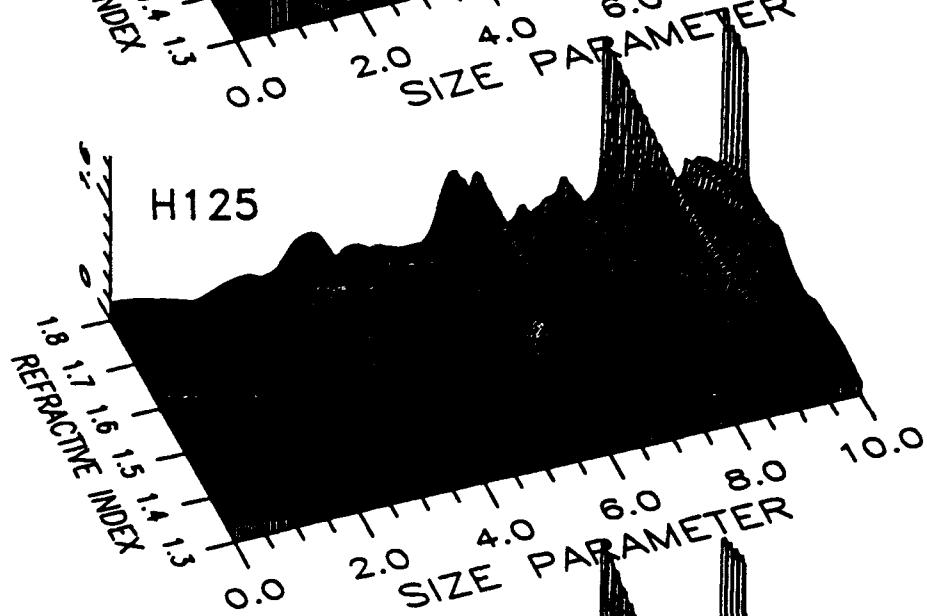
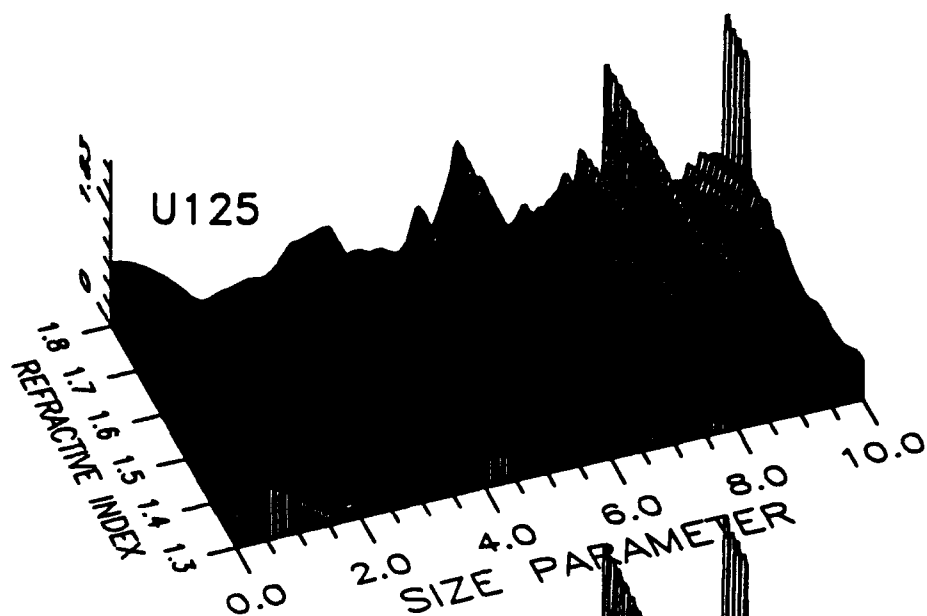


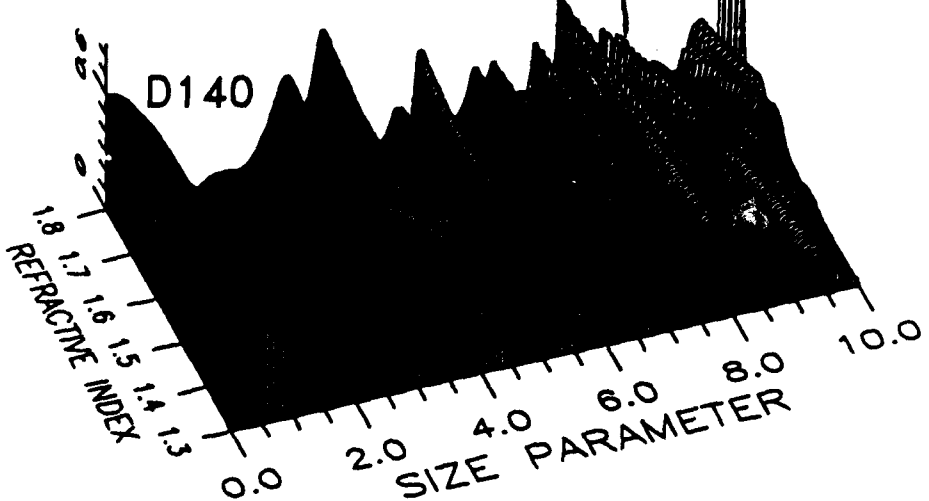
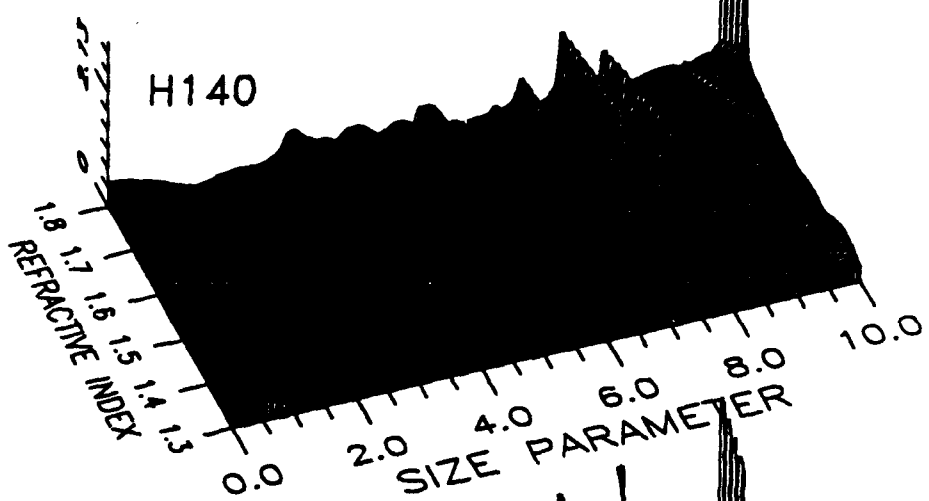
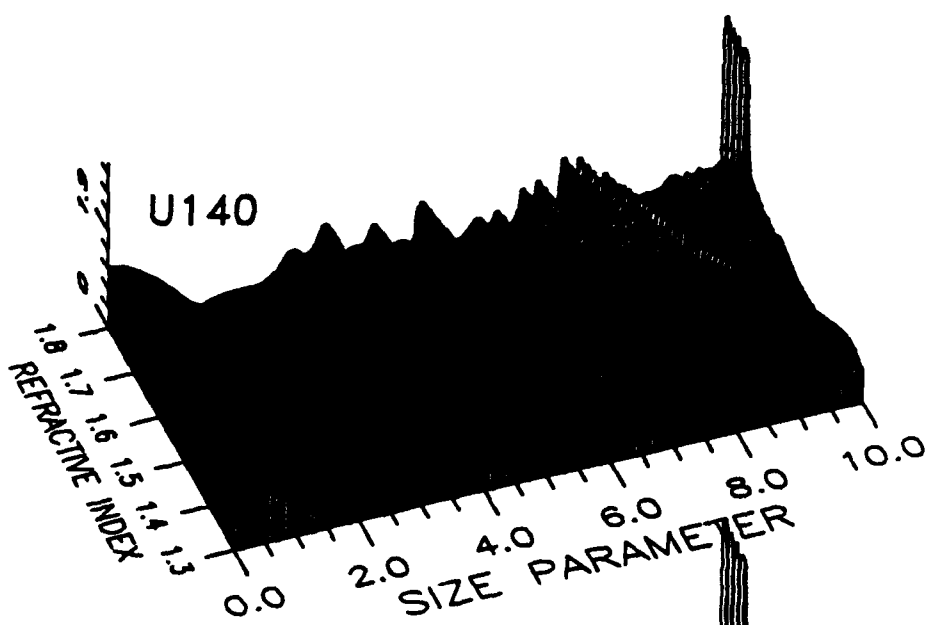


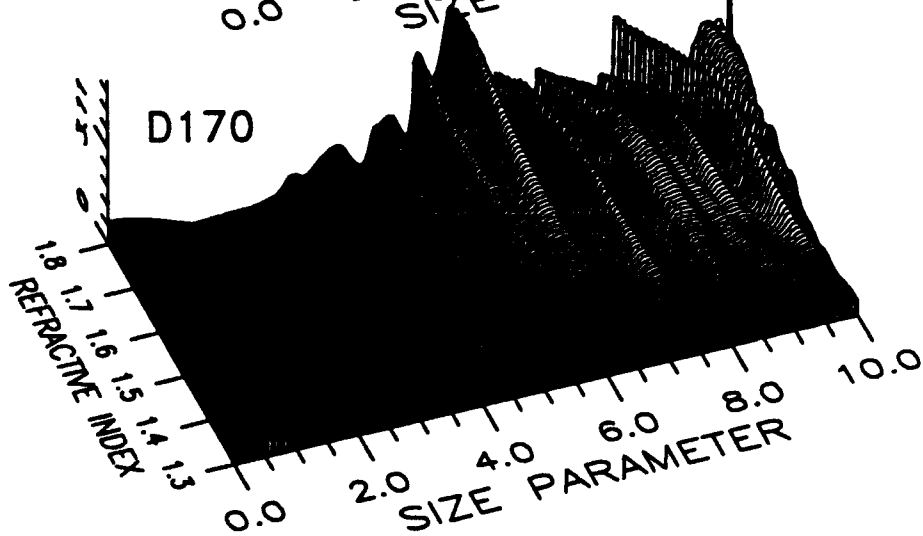
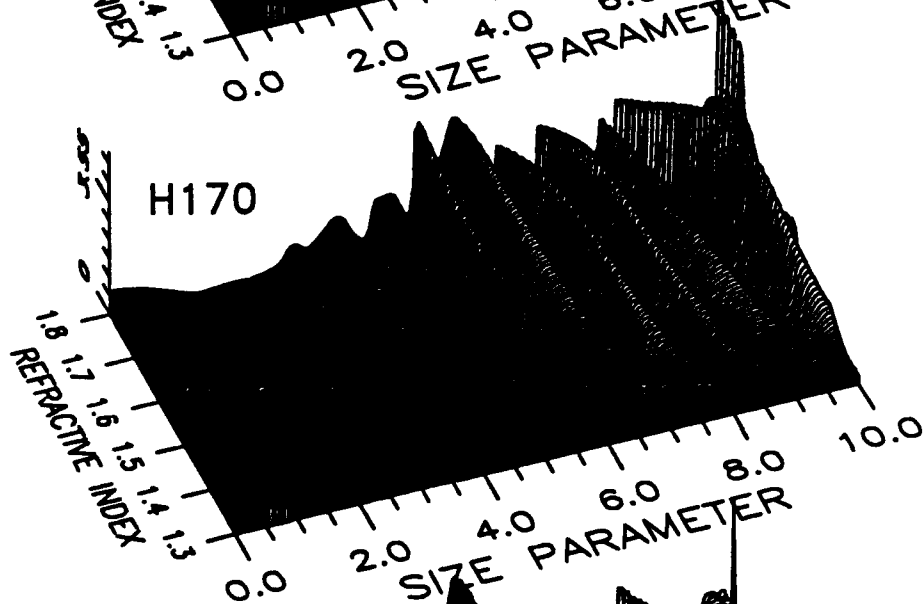
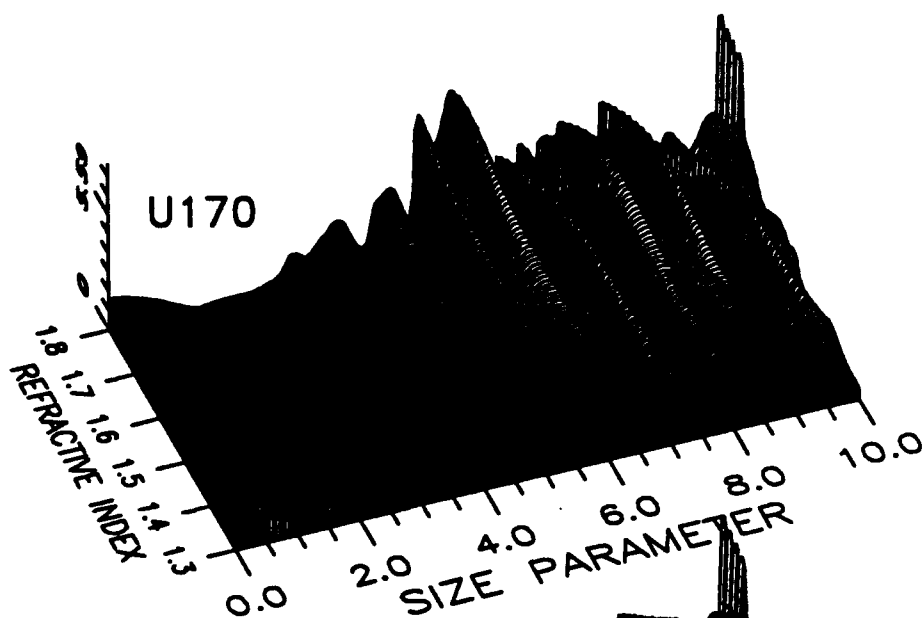












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APPENDIX C  
INVERT.F LISTING

PROGRAM		INVERT.F	
VERSION		Thu Jan 16 12:05:06 1992	
LINE #	SOURCE CODE	PAGE 1	
1	PROGRAM INVERT		
2	REAL ORDMIN(14,20200), ORDMAX(14,20200), EXPDAT(1000,25)		
3	REAL CALDAT(25), AVG, STD, SPX, SPHLIM, UNCAVG, UNCFIX		
4	REAL FLUX(14), UNC(14), HIVAL(14), LOVAL(14)		
5	INTEGER NDXMIN(14,20200), NDXMAX(14,20200), NPARTS		
6	INTEGER I, J, K, NUMCHN, HITS(20200), MISSES(20200)		
7	INTEGER MISLIM, ITRY, ILO, IHI, COUNT, DENS		
8	CHARACTER*12 ORNFIL(14), ORXFIL(14), NDNFIL(14), NDXFIL(14)		
9	CHARACTER*24 EXPNAM, OUTNAM, CALNAM, OLDNAM		
10	CHARACTER*7 DATE		
11			
12 C	Below, left side expressions are character variables used		
13 C	only in do loops to read in the previously calculated data.		
14 C	Right side strings are the file names containing the data.		
15			
16			
17	ORNFIL(1) = 'ORD_U040.MIN'		
18	ORXFIL(1) = 'ORD_U040.MAX'		
19	NDNFIL(1) = 'NDX_U040.MIN'		
20	NDXFIL(1) = 'NDX_U040.MAX'		
21			
22	ORNFIL(2) = 'ORD_U075.MIN'		
23	ORXFIL(2) = 'ORD_U075.MAX'		
24	NDNFIL(2) = 'NDX_U075.MIN'		
25	NDXFIL(2) = 'NDX_U075.MAX'		
26			
27	ORNFIL(3) = 'ORD_U090.MIN'		
28	ORXFIL(3) = 'ORD_U090.MAX'		
29	NDNFIL(3) = 'NDX_U090.MIN'		
30	NDXFIL(3) = 'NDX_U090.MAX'		
31			
32	ORNFIL(4) = 'ORD_U105.MIN'		
33	ORXFIL(4) = 'ORD_U105.MAX'		
34	NDNFIL(4) = 'NDX_U105.MIN'		
35	NDXFIL(4) = 'NDX_U105.MAX'		
36			
37	ORNFIL(5) = 'ORD_U125.MIN'		
38	ORXFIL(5) = 'ORD_U125.MAX'		
39	NDNFIL(5) = 'NDX_U125.MIN'		
40	NDXFIL(5) = 'NDX_U125.MAX'		
41			
42	ORNFIL(6) = 'ORD_U140.MIN'		
43	ORXFIL(6) = 'ORD_U140.MAX'		
44	NDNFIL(6) = 'NDX_U140.MIN'		
45	NDXFIL(6) = 'NDX_U140.MAX'		
46			
47	ORNFIL(7) = 'ORD_H040.MIN'		
48	ORXFIL(7) = 'ORD_H040.MAX'		
49	NDNFIL(7) = 'NDX_H040.MIN'		
50	NDXFIL(7) = 'NDX_H040.MAX'		
51			
52	ORNFIL(8) = 'ORD_H075.MIN'		
53	ORXFIL(8) = 'ORD_H075.MAX'		
54	NDNFIL(8) = 'NDX_H075.MIN'		
55	NDXFIL(8) = 'NDX_H075.MAX'		
56			
57	ORNFIL(9) = 'ORD_H090.MIN'		
58	ORXFIL(9) = 'ORD_H090.MAX'		
59	NDNFIL(9) = 'NDX_H090.MIN'		
60	NDXFIL(9) = 'NDX_H090.MAX'		

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LINE #	SOURCE CODE	PAGE 2
61		
62	ORNFIL(10) = 'ORD_H105.MIN'	
63	ORXFIL(10) = 'ORD_H105.MAX'	
64	NDNFIL(10) = 'NDX_H105.MIN'	
65	NDXFIL(10) = 'NDX_H105.MAX'	
66		
67	ORNFIL(11) = 'ORD_H125.MIN'	
68	ORXFIL(11) = 'ORD_H125.MAX'	
69	NDNFIL(11) = 'NDX_H125.MIN'	
70	NDXFIL(11) = 'NDX_H125.MAX'	
71		
72	ORNFIL(12) = 'ORD_H140.MIN'	
73	ORXFIL(12) = 'ORD_H140.MAX'	
74	NDNFIL(12) = 'NDX_H140.MIN'	
75	NDXFIL(12) = 'NDX_H140.MAX'	
76		
77	ORNFIL(13) = 'ORD_D040.MIN'	
78	ORXFIL(13) = 'ORD_D040.MAX'	
79	NDNFIL(13) = 'NDX_D040.MIN'	
80	NDXFIL(13) = 'NDX_D040.MAX'	
81		
82	ORNFIL(14) = 'ORD_D090.MIN'	
83	ORXFIL(14) = 'ORD_D090.MAX'	
84	NDNFIL(14) = 'NDX_D090.MIN'	
85	NDXFIL(14) = 'NDX_D090.MAX'	
86		
87		
88	C     Fill the array ORDMIN(14,20200) with previously calculated data	
89	DO 10 I=1,14	
90	OPEN (UNIT=3, FILE=ORNFIL(I),ACCESS='SEQUENTIAL',	
91	&     FORM='FORMATTED', STATUS='OLD')	
92	READ(3,*) (ORDMIN(I,J), J=1,20200)	
93	10 CONTINUE	
94	CLOSE (3)	
95		
96	C     Fill the array ORDMAX(14,20200) with previously calculated data	
97	DO 20 I=1,14	
98	OPEN (UNIT=3, FILE=ORXFIL(I),ACCESS='SEQUENTIAL',	
99	&     FORM='FORMATTED', STATUS='OLD')	
100	READ(3,*) (ORDMAX(I,J), J=1,20200)	
101	20 CONTINUE	
102	CLOSE (3)	
103		
104	C     Fill the array NOXMIN(14,20200) with previously calculated data	
105	DO 30 I=1,14	
106	OPEN (UNIT=3, FILE=NDNFIL(I),ACCESS='SEQUENTIAL',	
107	&     FORM='FORMATTED', STATUS='OLD')	
108	READ(3,*) (NOXMIN(I,J), J=1,20200)	
109	30 CONTINUE	
110	CLOSE (3)	
111		
112	C     Fill the array NOXMAX(14,20200) with previously calculated data	
113	DO 40 I=1,14	
114	OPEN (UNIT=3, FILE=NDXFIL(I),ACCESS='SEQUENTIAL',	
115	&     FORM='FORMATTED', STATUS='OLD')	
116	READ(3,*) (NOXMAX(I,J), J=1,20200)	
117	40 CONTINUE	
118	CLOSE (3)	
119	C     The previously calculated data is now all set up in RAM. Read	
120	C     in the experimental data from a group of ~500 particles, ie a	

PROGRAM

INVERT.F

VERSION

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LINE #	SOURCE CODE	PAGE 3
121 C	file outputted from TRANS.EXE such as E118A.PRN. The length	
122 C	of the filename cannot be known ahead of time, so it must be	
123 C	determined during runtime. The maximum length of the filename	
124 C	should not exceed 24 characters; I will also assume that the	
125 C	number of particles represented by the data does not exceed	
126 C	1000.	
127		
128	50 WRITE (*,*) ' ENTER PATH/FILE NAME OF DATA SET TO PROCESS'	
129	WRITE (*,*) ' EXAMPLES: I183.PRN or C:\WYATT\VI107B.PRN'	
130	WRITE (*,*) ' or enter x to quit program'	
131	READ (*, '(A)') EXPNAM	
132	IF ((EXPNAM(1:1) .EQ. 'X') .OR. (EXPNAM(1:1) .EQ. 'x')) THEN	
133	GO TO 270	
134	END IF	
135	OPEN (UNIT=3, FILE=EXPNAM, ACCESS='SEQUENTIAL',	
136	& FORM='FORMATTED', STATUS='OLD')	
137		
138		
139 C	Pause here to construct OUTNAM, the name of the output file	
140 C	which will be written at the end of this entire program. It	
141 C	will, by the construction of its name, go to whatever sub-	
142 C	directory the data set (EXPNAM) came from. In effect we will	
143 C	just substitute .MAP for .PRN in the string held by EXPNAM.	
144	I=1	
145	60 I=I+1	
146	IF (I .GE. 22) GO TO 50	
147	IF (EXPNAM(I:1) .NE. '.') GO TO 60	
148	OUTNAM = EXPNAM(1:1) // 'MAP'	
149 C	The "." is in the position corresponding to the current	
150 C	value of I. The total length of OUTNAM (and EXPNAM) is	
151 C	I+3 characters.	
152 C	Back to reading in the data:	
153		
154	DO 70 I=1,1000	
155	READ (3,*,END=80) (EXPDAT(I,J), J=1,25)	
156	70 CONTINUE	
157 C	Control should jump from the do-loop to statement 80 when EOF	
158 C	is reached, presumably before I=1000. When it exits the	
159 C	current value of I -1 should be the	
160 C	number of rows of data, ie., the number of particles in the	
161 C	data set (nparts).	
162	80 CLOSE(3)	
163	NPARTS = I-1	
164		
165 C	temporary	
166	WRITE (*,*) ' ENTER THE AMOUNT OF UNCERTAINTY TO BE ASSOCIATED'	
167	WRITE (*,*) ' WITH THIS THESE DATA. Enter as a decimal number'	
168	WRITE (*,*) ' from 0 to 1.0 ie, +/- 25% entered as 0.25'	
169	READ (*,*) UNCFIX	
170	DO 79 I=1,14	
171	UNC(I) = UNCFIX	
172	79 CONTINUE	
173		
174		
175		
176 C	Somewhere on disk I must have a file of correction factors	
177 C	previously determined in a calibration procedure and applicable	
178 C	to the experimental data which is here being analyzed. Those	
179 C	factors must be read in and multiplied against the corresponding	
180 C	columns of EXPDAT. Assume the format of the calibration file is	

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LINE #	SOURCE CODE	PAGE 4
181 C		
182 C	23Feb91 E1107A.PRM	
183 C	0 1	
184 C	1 1.0762	
185 C	2 0.8997	
186 C	.	
187 C	.	
188 C	22 1.677	
189 C	23 0.944	
190 C		
191 C	First line gives date of calibration and the data set (of	
192 C	spheres) used to perform the calibration. Thereafter the left	
193 C	column gives the fiber optic channel number and the right column	
194 C	the corresponding multiplicative correction factor. The	
195 C	channels labeled 0 and 15 are the bundles, and we'll just set	
196 C	the correction factor to 1. 25 lines in all.	
197 C		
198	WRITE (*,*) 'ENTER THE PATH/FILE NAME OF THE APPLICABLE'	
199	WRITE (*,*) 'CALIBRATION FILE. Enter L to just re-use the Latest'	
200	WRITE (*,*) 'filename used this session.'	
201	READ (*, '(A)') CALNAM	
202	IF ((CALNAM(1:1) .EQ. 'L') .OR. (CALNAM(1:1) .EQ. '1')) GO TO 85	
203	OLDNAM = CALNAM	
204	85 CALNAM = OLDNAM	
205	OPEN (UNIT=3, FILE=CALNAM, ACCESS='SEQUENTIAL',	
206	& FORM='FORMATTED', STATUS='OLD')	
207	READ (3, '(A)') DATE	
208	CALDAT(1) = 1.0	
209	DO 90 K=2,25	
210	READ(3,*) NUMCHN, CALDAT(K)	
211	90 CONTINUE	
212	CLOSE (3)	
213		
214 C	Now make the calibration correction:	
215	DO 100 I=1, NPARTS	
216	DO 110, K=1, 25	
217	EXPDAT(I,K) = EXPDAT(I,K)*CALDAT(K)	
218	110 CONTINUE	
219	100 CONTINUE	
220		
221 C	Now the array EXPDAT contains the corrected data values, ready	
222 C	for use.	
223		
224		
225 C	Initialize the group accumulator [HITS(20200)] to all zeros.	
226 C	This is the only time it will be zeroed; its status at the end	
227 C	of the program is the output we're looking for. Also initialize	
228 C	the particle accumulator [MISSES(20200)] for the first time; it	
229 C	will be reset to zero again at the end of each particle do-loop.	
230		
231	DO 120 J=1,20200	
232	HITS(J) = 0	
233	MISSES(J) = 0	
234	120 CONTINUE	
235		
236 C	Now begins the particle do-loop; ie, we look at particles one at	
237 C	a time (the Ith particle)	
238		
239	DO 200 I=1, NPARTS	
240		

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LINE #	SOURCE CODE	PAGE 5
241	AVG = (EXPDAT(I,13) + EXPDAT(I,14) + EXPDAT(I,15) + EXPDAT(I,16)	
242	& + EXPDAT(I,22) + EXPDAT(I,23) + EXPDAT(I,24) + EXPDAT(I,25))	
243	& /8.0	
244	STD =SQRT(((EXPDAT(I,13)-AVG)**2 + (EXPDAT(I,14)-AVG)**2	
245	& + (EXPDAT(I,15)-AVG)**2 + (EXPDAT(I,16)-AVG)**2	
246	& + (EXPDAT(I,22)-AVG)**2 + (EXPDAT(I,23)-AVG)**2	
247	& + (EXPDAT(I,24)-AVG)**2 + (EXPDAT(I,25)-AVG)**2)/8.0)	
248	SPX = 1.0 - (STD/(2.6458*AVG))	
249		
250		
251 C	If this particle isn't a good sphere, stop right now	
252	SPHLIM = 0.9	
253	IF (SPX .LT. SPHLIM) GO TO 200	
254		
255 C	The uncertainty to be associated with each data point (in	
256 C	EXPDAT) depends upon the magnitude of the data, generally	
257 C	getting worse as the intensity dims. I don't yet know how to	
258 C	calculate the uncertainty, but I will assume that it will be by	
259 C	exactly the same formula for all channels. Give the observables	
260 C	numbers (1-14) for identification. See page 14 hand notes.	
261		
262 C	UNCAVG = f{avg} not yet known	
263		
264	FLUX(1) = EXPDAT(I,11)	
265	FLUX(2) = EXPDAT(I,8)	
266	FLUX(3) = EXPDAT(I,9)	
267	FLUX(4) = EXPDAT(I,20)	
268	FLUX(5) = EXPDAT(I,5)	
269	FLUX(6) = EXPDAT(I,6)	
270	FLUX(7) = EXPDAT(I,10)	
271	FLUX(8) = EXPDAT(I,7)	
272	FLUX(9) = EXPDAT(I,19)	
273	FLUX(10) = EXPDAT(I,21)	
274	FLUX(11) = EXPDAT(I,3)	
275	FLUX(12) = EXPDAT(I,4)	
276	FLUX(13) = EXPDAT(I,12)	
277	FLUX(14) = EXPDAT(I,18)	
278		
279	DO 124 J=1,14	
280 C	UNC(J) = function of flux(j) still unknown	
281	HIVAL(J) = (FLUX(J)/AVG) * (1.0 + UNC(J))	
282	LOVAL(J) = (FLUX(J)/AVG) * (1.0 - UNC(J))	
283		
284	124 CONTINUE	
285		
286 C	Now we do a do-loop over the observables, writing to MISSES	
287 C	the result of each observable trial	
288		
289	DO 150 K=1,14	
290	ILO = 1	
291	IHI = 20200	
292	ITRY = 10100	
293	DO 130 COUNT=1,15	
294	IF (ORDMIN(K,ITRY) .LT. HIVAL(K)) THEN	
295	ILO = ITRY	
296	ITRY = INT((ITRY+IHI)/2)	
297	ELSE	
298	IHI = ITRY	
299	ITRY = INT((ITRY+ILO)/2)	
300	END IF	

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LINE #	SOURCE CODE	PAGE 6
301	130 CONTINUE	
302		
303		
304	C Now ITRY is the element of ORDMIN whose value equals HIVAL(K)	
305	DO 132 L=ITRY,20200	
306	MISSES(NDXMIN(K,L)) = MISSES(NDXMIN(K,L)) + 1	
307	132 CONTINUE	
308		
309	C Repeat the above for ORDMAX:	
310	ILO = 1	
311	IHI = 20200	
312	ITRY = 10100	
313	DO 134 COUNT=1,15	
314	IF (ORDMAX(K,ITRY) .LT. LOVAL(K)) THEN	
315	ILO = ITRY	
316	ITRY = INT((ITRY+IHI)/2)	
317	ELSE	
318	IHI = ITRY	
319	ITRY = INT((ITRY+ILO)/2)	
320	END IF	
321	134 CONTINUE	
322		
323	C This time at the end of the loop ITRY is the element of ORDMAX	
324	C whose value equals (closely enough) LOVAL. The elements of	
325	C NDXMAX from 1 up to ITRY contain the numbers (ie, names) of some	
326	C more missed pixels. Increment MISSES accordingly.	
327	DO 136 L=1,ITRY	
328	MISSES(NDXMAX(K,L)) = MISSES(NDXMAX(K,L)) + 1	
329	136 CONTINUE	
330	C This completes the incrementing of MISSES for this one (kth)	
331	C observable. Loop back for the next observable.	
332	150 CONTINUE	
333		
334	C The array MISSES is now filled, for this one particle. Each of	
335	C its 20200 elements contains an integer from 0 to 14, which	
336	C counts the number of times the corresponding pixel FAILED to be	
337	C in agreement with the data.	
338	C	
339	C Next step for this particle is to increment the array HITS. For	
340	C testing purposes, will tolerate three different levels of	
341	C hitting: eg. no misses, 1-2 misses, and 3-4 misses.	
342	C (Later, define only two levels of hitting: zero or 1 misses	
343	C and 2 or more misses)	
344	C	
345	C Whenever HITS is incremented, reset MISSES to zeros.	
346	C	
347	DO 160 J=1,20200	
348	IF (MISSES(J) .LE. 1) THEN	
349	HITS(J) = HITS(J) + 1	
350	END IF	
351	MISSES(J) = 0	
352	160 CONTINUE	
353		
354	C That does it for this particle, go back for the next one.	
355	200 CONTINUE	
356		
357	C Now all the particles have been analyzed, and HITS contains the	
358	C distribution over all particles (ie, each element of HITS	
359	C contains an integer which is the number of particles whose r and	
360	C n could have been the same as the pixel's r and n). Output the	

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LINE #	SOURCE CODE	PAGE 7
361	C array HITS - but sensibly; if there are no hits in a pixel, just	
362	C skip that pixel, don't write out a zero. DENS is a parameter	
363	C that will control how darkly a pixel square is printed under	
364	C PageGarden. First include EXPNAM and UNCFIX on picture	
365		
366	OPEN (UNIT=4, FILE=OUTNAM, ACCESS='SEQUENTIAL',	
367	& FORM='FORMATTED', STATUS='NEW')	
368		
369	WRITE(4,*) ' disp 4.5" 1.5" "TEST CASE:" '	
370	WRITE(4,201) EXPNAM	
371	201 FORMAT (' dispc " ',A,' ')	
372	WRITE(4,*) ' disp 4.5" 1.75" "UNCERTAINTY: +/- " '	
373	WRITE(4,202) 100.0*UNCFIX	
374	202 FORMAT (' dispc ",F4.1,'%')	
375		
376	DO 220 J=1,20200	
377	IF (HITS(J) .EQ. 0) THEN	
378	GO TO 220	
379	ELSE	
380	DENS = 60	
381	END IF	
382		
383	NPOSX = 525 + 12*MOD((J-1),200)	
384	NPOSY = 1870 - 12*INT((J-1)/200)	
385		
386	WRITE(4,250) NPOSX, NPOSY, DENS	
387	250 FORMAT(1X, 'area ',I4,'d ',I4,'d ', ' 12d 12d ',I3,/,	
388	& 1X, 'box +0 +0 12d 12d 1d')	
389		
390	220 CONTINUE	
391	CLOSE(4)	
392		
393	C Go back for another data set.	
394	GO TO 50	
395	270 STOP	
396	END	
397		